



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:31 PM UTC

PDB ID : 1VPX / pdb_00001vpx
Title : Crystal structure of Transaldolase (EC 2.2.1.2) (TM0295) from *Thermotoga maritima* at 2.40 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2004-11-23
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

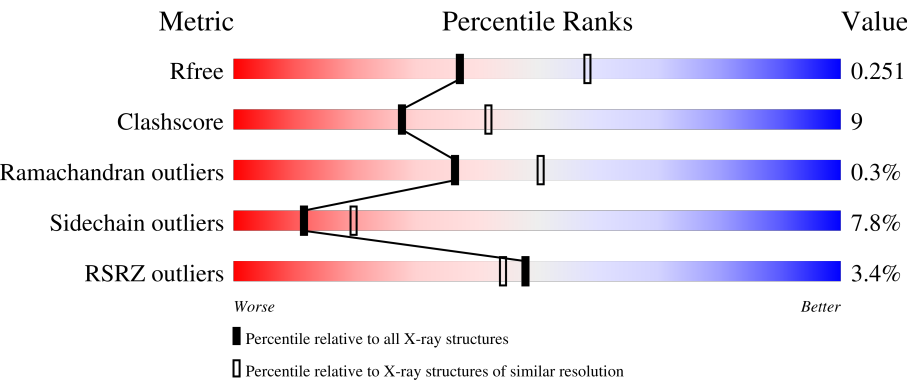
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	230	3% 71% 16% • 10%
1	B	230	5% 72% 17% • 9%
1	C	230	5% 67% 20% • 10%
1	D	230	% 72% 18% • 9%
1	E	230	% 67% 24% • 6%

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Mol	Chain	Length	Quality of chain
1	F	230	
1	G	230	
1	H	230	
1	I	230	
1	J	230	
1	K	230	
1	L	230	
1	M	230	
1	N	230	
1	O	230	
1	P	230	
1	Q	230	
1	R	230	
1	S	230	
1	T	230	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31916 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PROTEIN (Transaldolase (EC 2.2.1.2)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1591	1022	258	299	12			
1	B	209	Total	C	N	O	S	0	0	0
			1584	1016	260	296	12			
1	C	208	Total	C	N	O	S	0	0	0
			1560	997	252	299	12			
1	D	210	Total	C	N	O	S	0	0	0
			1615	1034	264	305	12			
1	E	216	Total	C	N	O	S	0	0	0
			1674	1075	272	315	12			
1	F	213	Total	C	N	O	S	0	0	0
			1655	1064	270	309	12			
1	G	216	Total	C	N	O	S	0	0	0
			1667	1070	271	314	12			
1	H	205	Total	C	N	O	S	0	0	0
			1550	996	248	294	12			
1	I	211	Total	C	N	O	S	0	0	0
			1615	1034	264	305	12			
1	J	213	Total	C	N	O	S	0	0	0
			1619	1038	263	306	12			
1	K	216	Total	C	N	O	S	0	0	0
			1651	1059	265	315	12			
1	L	204	Total	C	N	O	S	0	0	0
			1530	980	249	289	12			
1	M	198	Total	C	N	O	S	0	0	0
			1457	928	240	278	11			
1	N	204	Total	C	N	O	S	0	0	0
			1475	939	243	281	12			
1	O	210	Total	C	N	O	S	0	0	0
			1604	1025	260	307	12			
1	P	209	Total	C	N	O	S	0	0	0
			1576	1010	258	296	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	208	Total	C	N	O	S	0	1	0
			1596	1027	259	298	12			
1	R	210	Total	C	N	O	S	0	0	0
			1585	1014	259	300	12			
1	S	205	Total	C	N	O	S	0	0	0
			1533	978	254	290	11			
1	T	204	Total	C	N	O	S	0	0	0
			1541	987	249	293	12			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9WYD1
A	-10	GLY	-	expression tag	UNP Q9WYD1
A	-9	SER	-	expression tag	UNP Q9WYD1
A	-8	ASP	-	expression tag	UNP Q9WYD1
A	-7	LYS	-	expression tag	UNP Q9WYD1
A	-6	ILE	-	expression tag	UNP Q9WYD1
A	-5	HIS	-	expression tag	UNP Q9WYD1
A	-4	HIS	-	expression tag	UNP Q9WYD1
A	-3	HIS	-	expression tag	UNP Q9WYD1
A	-2	HIS	-	expression tag	UNP Q9WYD1
A	-1	HIS	-	expression tag	UNP Q9WYD1
A	0	HIS	-	expression tag	UNP Q9WYD1
B	-11	MET	-	expression tag	UNP Q9WYD1
B	-10	GLY	-	expression tag	UNP Q9WYD1
B	-9	SER	-	expression tag	UNP Q9WYD1
B	-8	ASP	-	expression tag	UNP Q9WYD1
B	-7	LYS	-	expression tag	UNP Q9WYD1
B	-6	ILE	-	expression tag	UNP Q9WYD1
B	-5	HIS	-	expression tag	UNP Q9WYD1
B	-4	HIS	-	expression tag	UNP Q9WYD1
B	-3	HIS	-	expression tag	UNP Q9WYD1
B	-2	HIS	-	expression tag	UNP Q9WYD1
B	-1	HIS	-	expression tag	UNP Q9WYD1
B	0	HIS	-	expression tag	UNP Q9WYD1
C	-11	MET	-	expression tag	UNP Q9WYD1
C	-10	GLY	-	expression tag	UNP Q9WYD1
C	-9	SER	-	expression tag	UNP Q9WYD1
C	-8	ASP	-	expression tag	UNP Q9WYD1
C	-7	LYS	-	expression tag	UNP Q9WYD1
C	-6	ILE	-	expression tag	UNP Q9WYD1
C	-5	HIS	-	expression tag	UNP Q9WYD1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP Q9WYD1
C	-3	HIS	-	expression tag	UNP Q9WYD1
C	-2	HIS	-	expression tag	UNP Q9WYD1
C	-1	HIS	-	expression tag	UNP Q9WYD1
C	0	HIS	-	expression tag	UNP Q9WYD1
D	-11	MET	-	expression tag	UNP Q9WYD1
D	-10	GLY	-	expression tag	UNP Q9WYD1
D	-9	SER	-	expression tag	UNP Q9WYD1
D	-8	ASP	-	expression tag	UNP Q9WYD1
D	-7	LYS	-	expression tag	UNP Q9WYD1
D	-6	ILE	-	expression tag	UNP Q9WYD1
D	-5	HIS	-	expression tag	UNP Q9WYD1
D	-4	HIS	-	expression tag	UNP Q9WYD1
D	-3	HIS	-	expression tag	UNP Q9WYD1
D	-2	HIS	-	expression tag	UNP Q9WYD1
D	-1	HIS	-	expression tag	UNP Q9WYD1
D	0	HIS	-	expression tag	UNP Q9WYD1
E	-11	MET	-	expression tag	UNP Q9WYD1
E	-10	GLY	-	expression tag	UNP Q9WYD1
E	-9	SER	-	expression tag	UNP Q9WYD1
E	-8	ASP	-	expression tag	UNP Q9WYD1
E	-7	LYS	-	expression tag	UNP Q9WYD1
E	-6	ILE	-	expression tag	UNP Q9WYD1
E	-5	HIS	-	expression tag	UNP Q9WYD1
E	-4	HIS	-	expression tag	UNP Q9WYD1
E	-3	HIS	-	expression tag	UNP Q9WYD1
E	-2	HIS	-	expression tag	UNP Q9WYD1
E	-1	HIS	-	expression tag	UNP Q9WYD1
E	0	HIS	-	expression tag	UNP Q9WYD1
F	-11	MET	-	expression tag	UNP Q9WYD1
F	-10	GLY	-	expression tag	UNP Q9WYD1
F	-9	SER	-	expression tag	UNP Q9WYD1
F	-8	ASP	-	expression tag	UNP Q9WYD1
F	-7	LYS	-	expression tag	UNP Q9WYD1
F	-6	ILE	-	expression tag	UNP Q9WYD1
F	-5	HIS	-	expression tag	UNP Q9WYD1
F	-4	HIS	-	expression tag	UNP Q9WYD1
F	-3	HIS	-	expression tag	UNP Q9WYD1
F	-2	HIS	-	expression tag	UNP Q9WYD1
F	-1	HIS	-	expression tag	UNP Q9WYD1
F	0	HIS	-	expression tag	UNP Q9WYD1
G	-11	MET	-	expression tag	UNP Q9WYD1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-10	GLY	-	expression tag	UNP Q9WYD1
G	-9	SER	-	expression tag	UNP Q9WYD1
G	-8	ASP	-	expression tag	UNP Q9WYD1
G	-7	LYS	-	expression tag	UNP Q9WYD1
G	-6	ILE	-	expression tag	UNP Q9WYD1
G	-5	HIS	-	expression tag	UNP Q9WYD1
G	-4	HIS	-	expression tag	UNP Q9WYD1
G	-3	HIS	-	expression tag	UNP Q9WYD1
G	-2	HIS	-	expression tag	UNP Q9WYD1
G	-1	HIS	-	expression tag	UNP Q9WYD1
G	0	HIS	-	expression tag	UNP Q9WYD1
H	-11	MET	-	expression tag	UNP Q9WYD1
H	-10	GLY	-	expression tag	UNP Q9WYD1
H	-9	SER	-	expression tag	UNP Q9WYD1
H	-8	ASP	-	expression tag	UNP Q9WYD1
H	-7	LYS	-	expression tag	UNP Q9WYD1
H	-6	ILE	-	expression tag	UNP Q9WYD1
H	-5	HIS	-	expression tag	UNP Q9WYD1
H	-4	HIS	-	expression tag	UNP Q9WYD1
H	-3	HIS	-	expression tag	UNP Q9WYD1
H	-2	HIS	-	expression tag	UNP Q9WYD1
H	-1	HIS	-	expression tag	UNP Q9WYD1
H	0	HIS	-	expression tag	UNP Q9WYD1
I	-11	MET	-	expression tag	UNP Q9WYD1
I	-10	GLY	-	expression tag	UNP Q9WYD1
I	-9	SER	-	expression tag	UNP Q9WYD1
I	-8	ASP	-	expression tag	UNP Q9WYD1
I	-7	LYS	-	expression tag	UNP Q9WYD1
I	-6	ILE	-	expression tag	UNP Q9WYD1
I	-5	HIS	-	expression tag	UNP Q9WYD1
I	-4	HIS	-	expression tag	UNP Q9WYD1
I	-3	HIS	-	expression tag	UNP Q9WYD1
I	-2	HIS	-	expression tag	UNP Q9WYD1
I	-1	HIS	-	expression tag	UNP Q9WYD1
I	0	HIS	-	expression tag	UNP Q9WYD1
J	-11	MET	-	expression tag	UNP Q9WYD1
J	-10	GLY	-	expression tag	UNP Q9WYD1
J	-9	SER	-	expression tag	UNP Q9WYD1
J	-8	ASP	-	expression tag	UNP Q9WYD1
J	-7	LYS	-	expression tag	UNP Q9WYD1
J	-6	ILE	-	expression tag	UNP Q9WYD1
J	-5	HIS	-	expression tag	UNP Q9WYD1

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-4	HIS	-	expression tag	UNP Q9WYD1
J	-3	HIS	-	expression tag	UNP Q9WYD1
J	-2	HIS	-	expression tag	UNP Q9WYD1
J	-1	HIS	-	expression tag	UNP Q9WYD1
J	0	HIS	-	expression tag	UNP Q9WYD1
K	-11	MET	-	expression tag	UNP Q9WYD1
K	-10	GLY	-	expression tag	UNP Q9WYD1
K	-9	SER	-	expression tag	UNP Q9WYD1
K	-8	ASP	-	expression tag	UNP Q9WYD1
K	-7	LYS	-	expression tag	UNP Q9WYD1
K	-6	ILE	-	expression tag	UNP Q9WYD1
K	-5	HIS	-	expression tag	UNP Q9WYD1
K	-4	HIS	-	expression tag	UNP Q9WYD1
K	-3	HIS	-	expression tag	UNP Q9WYD1
K	-2	HIS	-	expression tag	UNP Q9WYD1
K	-1	HIS	-	expression tag	UNP Q9WYD1
K	0	HIS	-	expression tag	UNP Q9WYD1
L	-11	MET	-	expression tag	UNP Q9WYD1
L	-10	GLY	-	expression tag	UNP Q9WYD1
L	-9	SER	-	expression tag	UNP Q9WYD1
L	-8	ASP	-	expression tag	UNP Q9WYD1
L	-7	LYS	-	expression tag	UNP Q9WYD1
L	-6	ILE	-	expression tag	UNP Q9WYD1
L	-5	HIS	-	expression tag	UNP Q9WYD1
L	-4	HIS	-	expression tag	UNP Q9WYD1
L	-3	HIS	-	expression tag	UNP Q9WYD1
L	-2	HIS	-	expression tag	UNP Q9WYD1
L	-1	HIS	-	expression tag	UNP Q9WYD1
L	0	HIS	-	expression tag	UNP Q9WYD1
M	-11	MET	-	expression tag	UNP Q9WYD1
M	-10	GLY	-	expression tag	UNP Q9WYD1
M	-9	SER	-	expression tag	UNP Q9WYD1
M	-8	ASP	-	expression tag	UNP Q9WYD1
M	-7	LYS	-	expression tag	UNP Q9WYD1
M	-6	ILE	-	expression tag	UNP Q9WYD1
M	-5	HIS	-	expression tag	UNP Q9WYD1
M	-4	HIS	-	expression tag	UNP Q9WYD1
M	-3	HIS	-	expression tag	UNP Q9WYD1
M	-2	HIS	-	expression tag	UNP Q9WYD1
M	-1	HIS	-	expression tag	UNP Q9WYD1
M	0	HIS	-	expression tag	UNP Q9WYD1
N	-11	MET	-	expression tag	UNP Q9WYD1

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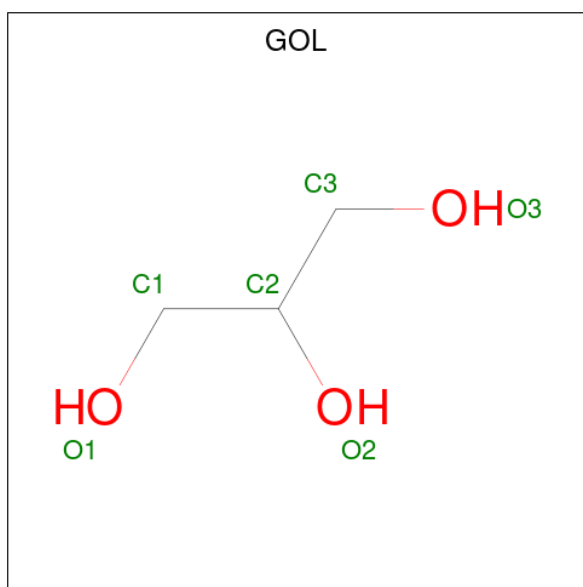
Chain	Residue	Modelled	Actual	Comment	Reference
N	-10	GLY	-	expression tag	UNP Q9WYD1
N	-9	SER	-	expression tag	UNP Q9WYD1
N	-8	ASP	-	expression tag	UNP Q9WYD1
N	-7	LYS	-	expression tag	UNP Q9WYD1
N	-6	ILE	-	expression tag	UNP Q9WYD1
N	-5	HIS	-	expression tag	UNP Q9WYD1
N	-4	HIS	-	expression tag	UNP Q9WYD1
N	-3	HIS	-	expression tag	UNP Q9WYD1
N	-2	HIS	-	expression tag	UNP Q9WYD1
N	-1	HIS	-	expression tag	UNP Q9WYD1
N	0	HIS	-	expression tag	UNP Q9WYD1
O	-11	MET	-	expression tag	UNP Q9WYD1
O	-10	GLY	-	expression tag	UNP Q9WYD1
O	-9	SER	-	expression tag	UNP Q9WYD1
O	-8	ASP	-	expression tag	UNP Q9WYD1
O	-7	LYS	-	expression tag	UNP Q9WYD1
O	-6	ILE	-	expression tag	UNP Q9WYD1
O	-5	HIS	-	expression tag	UNP Q9WYD1
O	-4	HIS	-	expression tag	UNP Q9WYD1
O	-3	HIS	-	expression tag	UNP Q9WYD1
O	-2	HIS	-	expression tag	UNP Q9WYD1
O	-1	HIS	-	expression tag	UNP Q9WYD1
O	0	HIS	-	expression tag	UNP Q9WYD1
P	-11	MET	-	expression tag	UNP Q9WYD1
P	-10	GLY	-	expression tag	UNP Q9WYD1
P	-9	SER	-	expression tag	UNP Q9WYD1
P	-8	ASP	-	expression tag	UNP Q9WYD1
P	-7	LYS	-	expression tag	UNP Q9WYD1
P	-6	ILE	-	expression tag	UNP Q9WYD1
P	-5	HIS	-	expression tag	UNP Q9WYD1
P	-4	HIS	-	expression tag	UNP Q9WYD1
P	-3	HIS	-	expression tag	UNP Q9WYD1
P	-2	HIS	-	expression tag	UNP Q9WYD1
P	-1	HIS	-	expression tag	UNP Q9WYD1
P	0	HIS	-	expression tag	UNP Q9WYD1
Q	-11	MET	-	expression tag	UNP Q9WYD1
Q	-10	GLY	-	expression tag	UNP Q9WYD1
Q	-9	SER	-	expression tag	UNP Q9WYD1
Q	-8	ASP	-	expression tag	UNP Q9WYD1
Q	-7	LYS	-	expression tag	UNP Q9WYD1
Q	-6	ILE	-	expression tag	UNP Q9WYD1
Q	-5	HIS	-	expression tag	UNP Q9WYD1

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-4	HIS	-	expression tag	UNP Q9WYD1
Q	-3	HIS	-	expression tag	UNP Q9WYD1
Q	-2	HIS	-	expression tag	UNP Q9WYD1
Q	-1	HIS	-	expression tag	UNP Q9WYD1
Q	0	HIS	-	expression tag	UNP Q9WYD1
R	-11	MET	-	expression tag	UNP Q9WYD1
R	-10	GLY	-	expression tag	UNP Q9WYD1
R	-9	SER	-	expression tag	UNP Q9WYD1
R	-8	ASP	-	expression tag	UNP Q9WYD1
R	-7	LYS	-	expression tag	UNP Q9WYD1
R	-6	ILE	-	expression tag	UNP Q9WYD1
R	-5	HIS	-	expression tag	UNP Q9WYD1
R	-4	HIS	-	expression tag	UNP Q9WYD1
R	-3	HIS	-	expression tag	UNP Q9WYD1
R	-2	HIS	-	expression tag	UNP Q9WYD1
R	-1	HIS	-	expression tag	UNP Q9WYD1
R	0	HIS	-	expression tag	UNP Q9WYD1
S	-11	MET	-	expression tag	UNP Q9WYD1
S	-10	GLY	-	expression tag	UNP Q9WYD1
S	-9	SER	-	expression tag	UNP Q9WYD1
S	-8	ASP	-	expression tag	UNP Q9WYD1
S	-7	LYS	-	expression tag	UNP Q9WYD1
S	-6	ILE	-	expression tag	UNP Q9WYD1
S	-5	HIS	-	expression tag	UNP Q9WYD1
S	-4	HIS	-	expression tag	UNP Q9WYD1
S	-3	HIS	-	expression tag	UNP Q9WYD1
S	-2	HIS	-	expression tag	UNP Q9WYD1
S	-1	HIS	-	expression tag	UNP Q9WYD1
S	0	HIS	-	expression tag	UNP Q9WYD1
T	-11	MET	-	expression tag	UNP Q9WYD1
T	-10	GLY	-	expression tag	UNP Q9WYD1
T	-9	SER	-	expression tag	UNP Q9WYD1
T	-8	ASP	-	expression tag	UNP Q9WYD1
T	-7	LYS	-	expression tag	UNP Q9WYD1
T	-6	ILE	-	expression tag	UNP Q9WYD1
T	-5	HIS	-	expression tag	UNP Q9WYD1
T	-4	HIS	-	expression tag	UNP Q9WYD1
T	-3	HIS	-	expression tag	UNP Q9WYD1
T	-2	HIS	-	expression tag	UNP Q9WYD1
T	-1	HIS	-	expression tag	UNP Q9WYD1
T	0	HIS	-	expression tag	UNP Q9WYD1

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



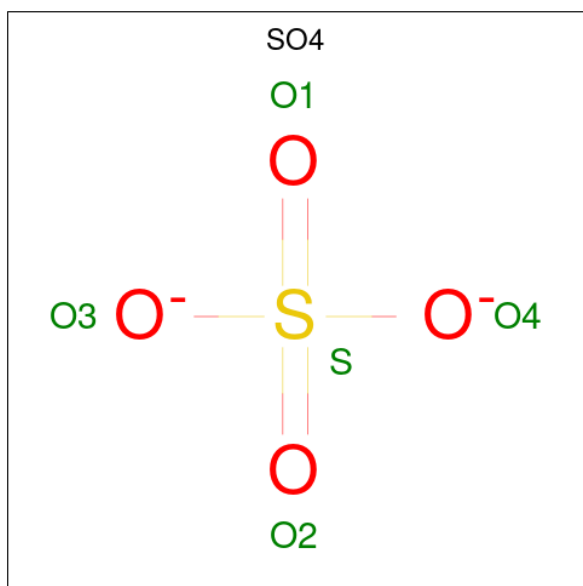
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	1
			10	5	5		
2	L	1	Total	C	O	0	0
			6	3	3		
2	M	1	Total	C	O	0	0
			6	3	3		
2	N	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	C	O	0	0
			6	3	3		
2	P	1	Total	C	O	0	0
			6	3	3		
2	P	1	Total	C	O	0	0
			6	3	3		
2	Q	1	Total	C	O	0	0
			6	3	3		
2	R	1	Total	C	O	0	0
			6	3	3		
2	S	1	Total	C	O	0	0
			6	3	3		
2	T	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		

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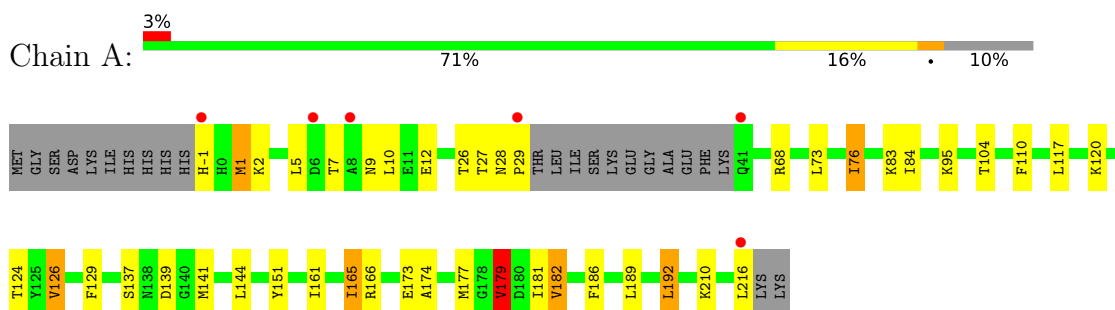
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	6	Total O 6 6	0	0
4	C	7	Total O 7 7	0	0
4	D	16	Total O 16 16	0	0
4	E	7	Total O 7 7	0	0
4	F	5	Total O 5 5	0	0
4	G	17	Total O 17 17	0	0
4	H	3	Total O 3 3	0	0
4	I	4	Total O 4 4	0	0
4	J	7	Total O 7 7	0	0
4	K	3	Total O 3 3	0	0
4	L	1	Total O 1 1	0	0
4	M	2	Total O 2 2	0	0
4	O	5	Total O 5 5	0	0
4	P	3	Total O 3 3	0	0
4	Q	7	Total O 7 7	0	0
4	R	2	Total O 2 2	0	0
4	S	2	Total O 2 2	0	0
4	T	1	Total O 1 1	0	0

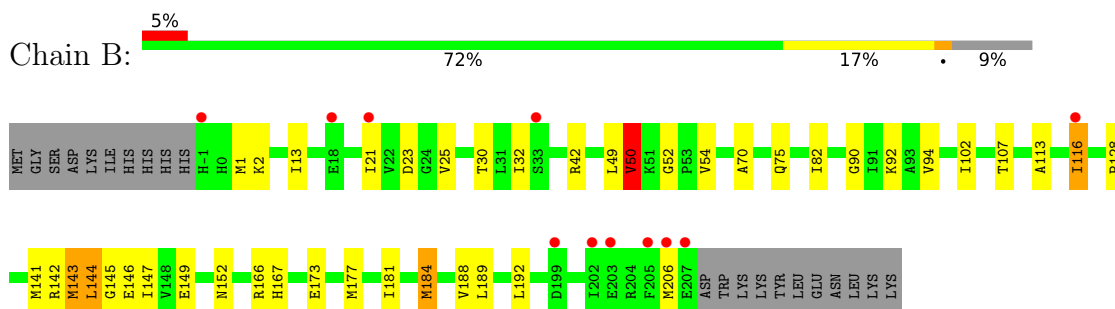
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

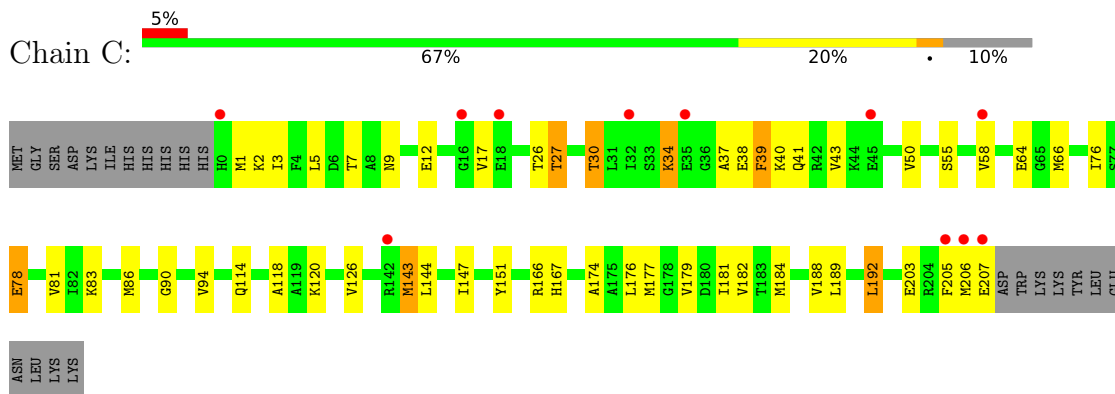
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))

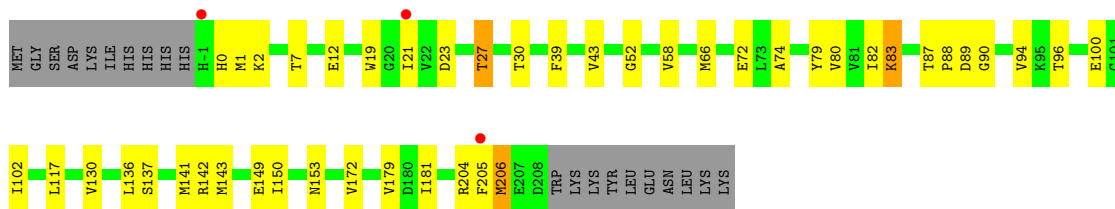


- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))

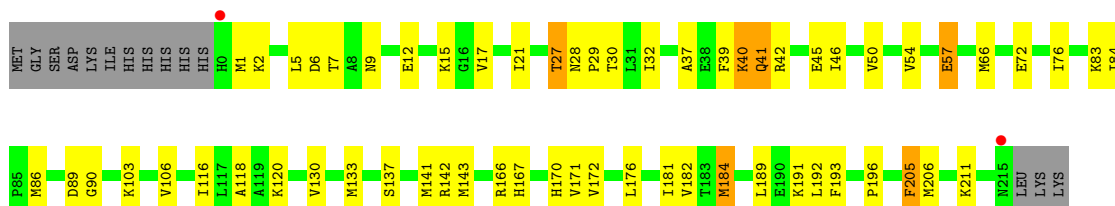


- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))

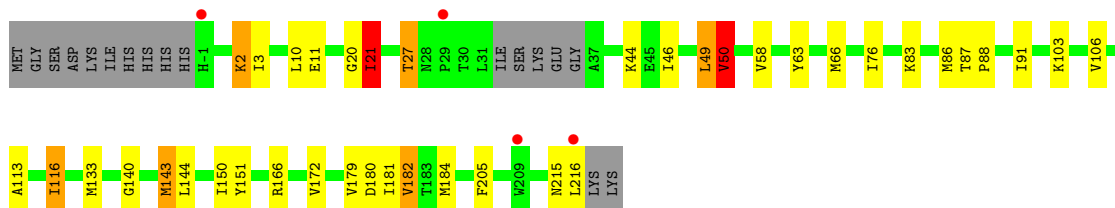
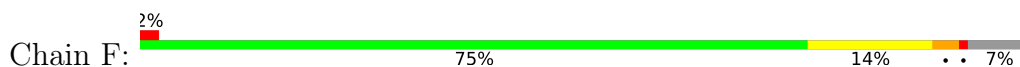




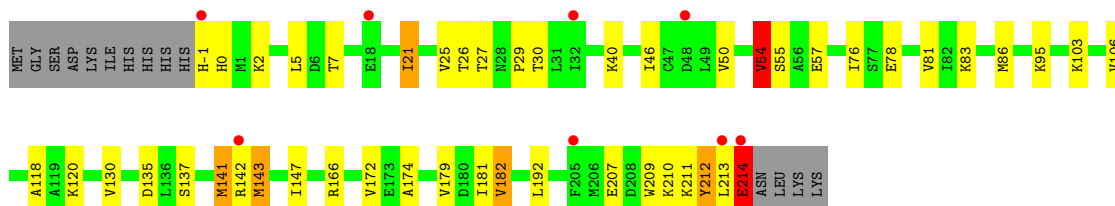
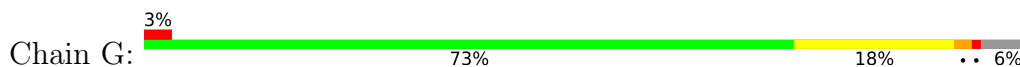
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



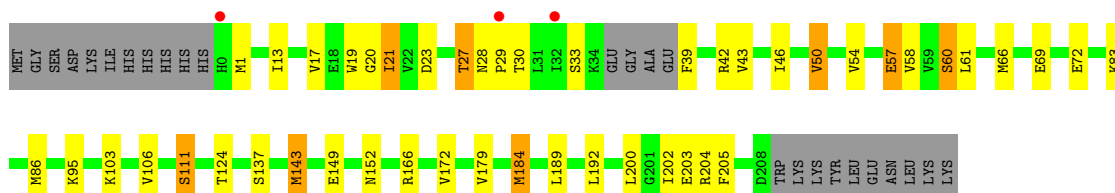
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))

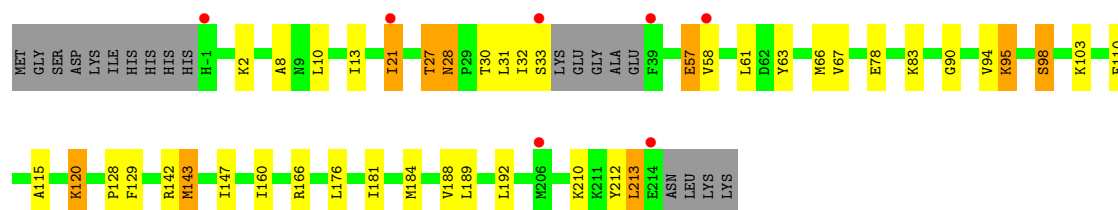


- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



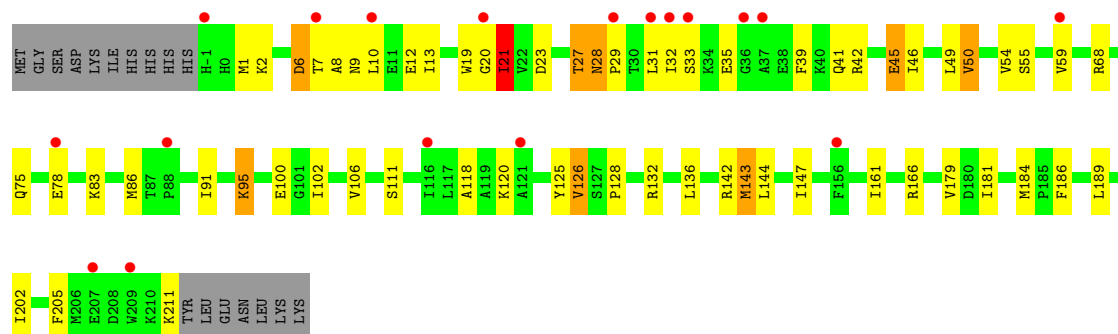
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))

Chain I: 



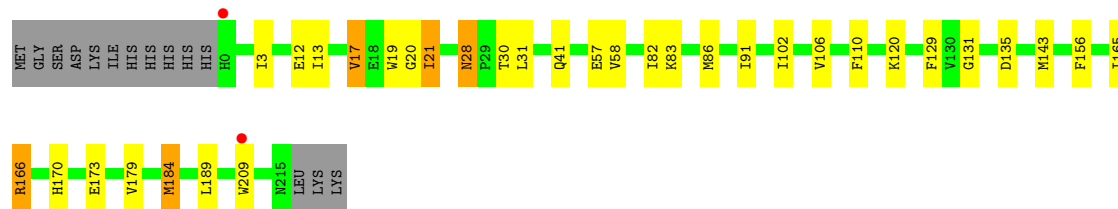
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))

Chain J: 



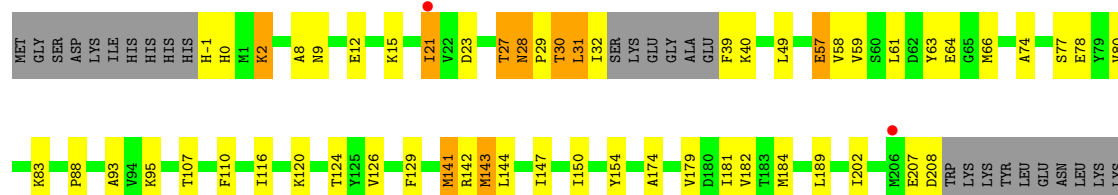
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))

Chain K: 

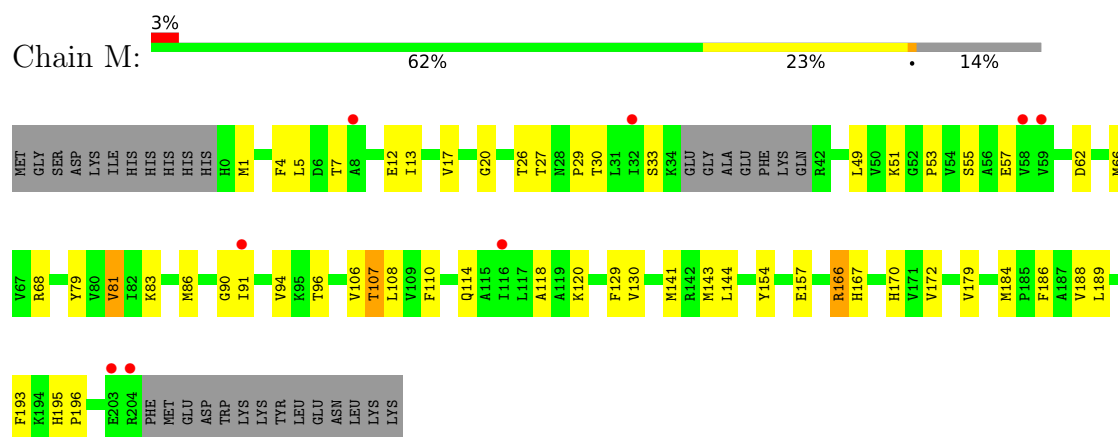


- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))

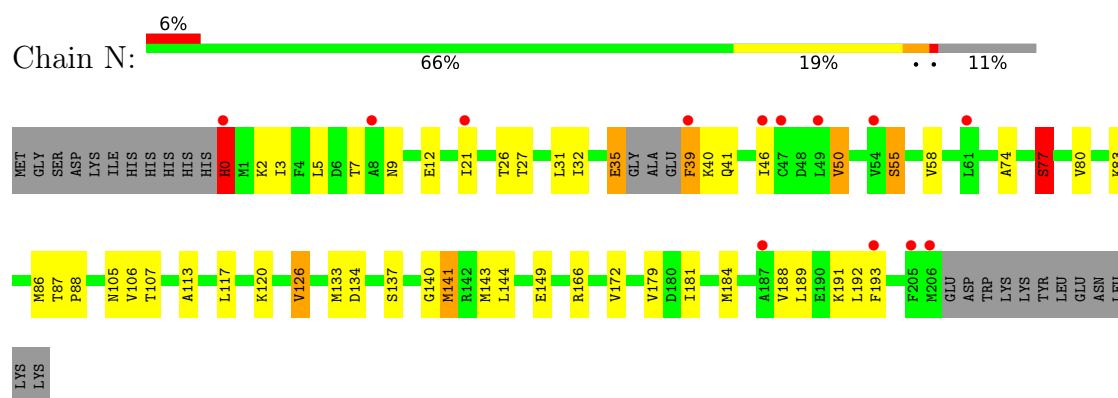
Chain L: 



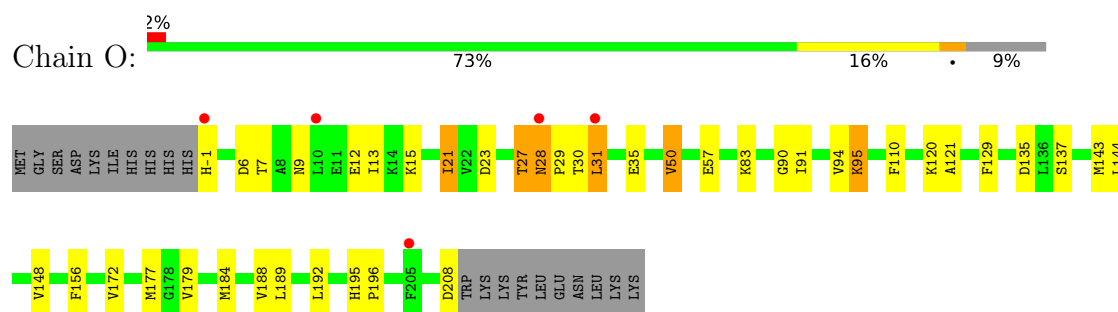
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



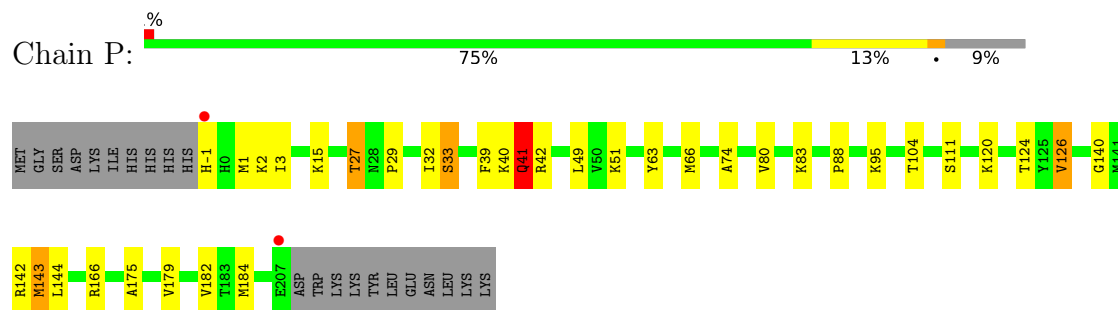
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



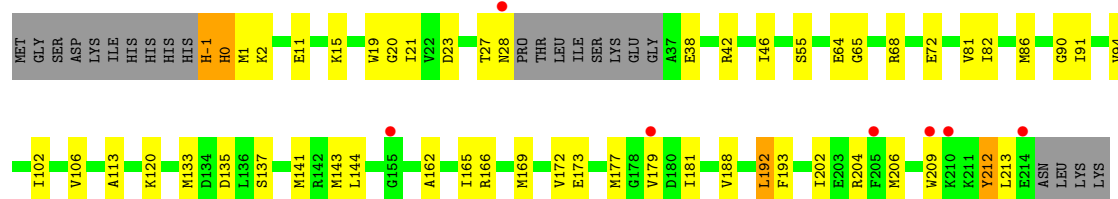
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



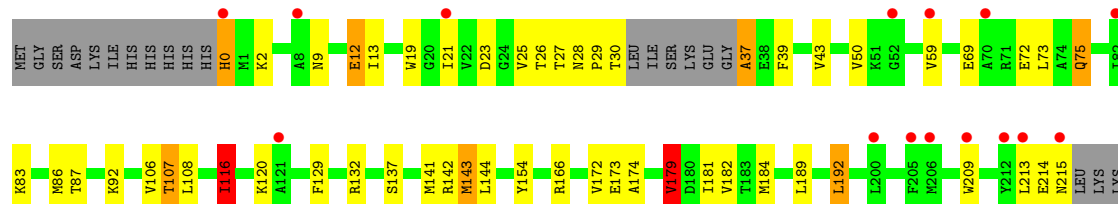
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



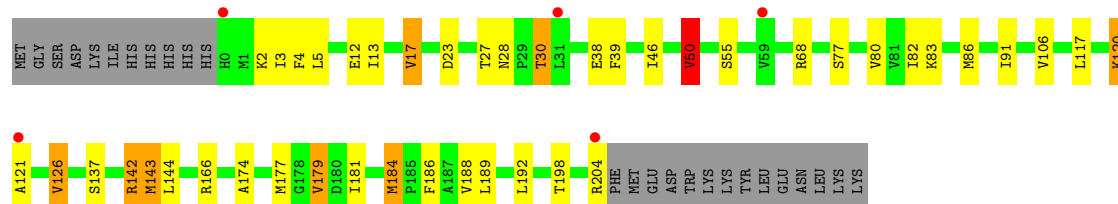
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



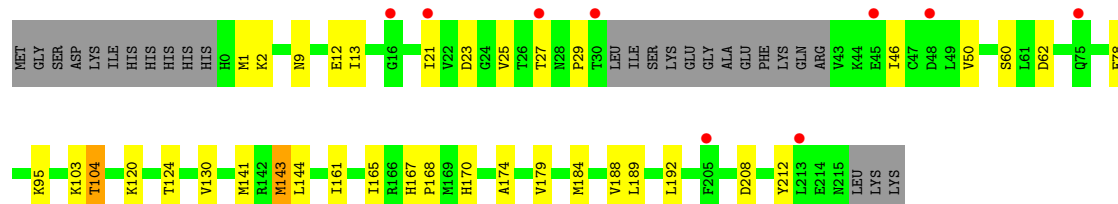
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	145.30Å 104.42Å 171.12Å 90.00° 108.99° 90.00°	Depositor
Resolution (Å)	83.13 – 2.40 83.13 – 2.40	Depositor EDS
% Data completeness (in resolution range)	85.9 (83.13-2.40) 85.6 (83.13-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.196 , 0.247 0.204 , 0.251	Depositor DCC
R_{free} test set	8140 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 71.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31916	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.93	1/1620 (0.1%)	1.06	2/2194 (0.1%)
1	B	0.97	0/1612	1.02	2/2182 (0.1%)
1	C	0.99	3/1586 (0.2%)	1.05	1/2147 (0.0%)
1	D	1.05	2/1643 (0.1%)	1.06	2/2223 (0.1%)
1	E	1.04	3/1704 (0.2%)	1.11	0/2305
1	F	0.94	1/1685 (0.1%)	1.08	2/2280 (0.1%)
1	G	1.22	3/1698 (0.2%)	1.12	3/2300 (0.1%)
1	H	0.97	0/1576	1.03	2/2136 (0.1%)
1	I	0.99	3/1643 (0.2%)	1.06	1/2226 (0.0%)
1	J	1.19	4/1649 (0.2%)	1.12	4/2236 (0.2%)
1	K	0.85	1/1681 (0.1%)	0.95	1/2279 (0.0%)
1	L	0.76	0/1556	0.98	2/2111 (0.1%)
1	M	0.78	0/1481	0.96	1/2009 (0.0%)
1	N	1.36	12/1498 (0.8%)	1.10	8/2027 (0.4%)
1	O	0.98	1/1632 (0.1%)	1.03	2/2209 (0.1%)
1	P	0.92	0/1603	1.01	1/2172 (0.0%)
1	Q	0.87	2/1625 (0.1%)	1.01	3/2200 (0.1%)
1	R	0.88	2/1613 (0.1%)	1.00	4/2188 (0.2%)
1	S	0.85	1/1559 (0.1%)	1.02	2/2112 (0.1%)
1	T	0.78	0/1569	0.94	0/2128
All	All	0.98	39/32233 (0.1%)	1.04	43/43664 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
1	N	0	1
1	R	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	214	GLU	C-O	21.96	1.67	1.23
1	J	45	GLU	CD-OE2	18.64	1.60	1.25
1	N	41	GLN	C-N	17.55	1.57	1.33
1	J	45	GLU	CD-OE1	16.76	1.57	1.25
1	N	41	GLN	C-O	16.31	1.43	1.24
1	N	39	PHE	N-CA	15.96	1.76	1.46
1	N	39	PHE	C-O	14.09	1.51	1.23
1	N	41	GLN	CA-C	11.99	1.69	1.52
1	N	40	LYS	C-O	11.94	1.39	1.24
1	N	40	LYS	C-N	11.71	1.49	1.33
1	N	35	GLU	CD-OE1	11.24	1.46	1.25
1	R	37	ALA	C-O	10.14	1.43	1.23
1	C	37	ALA	C-O	10.10	1.36	1.23
1	N	39	PHE	C-N	9.16	1.46	1.33
1	R	37	ALA	C-N	9.00	1.46	1.33
1	J	211	LYS	C-O	7.59	1.38	1.23
1	J	41	GLN	C-O	7.22	1.32	1.24
1	S	179	VAL	CA-CB	6.70	1.60	1.54
1	N	35	GLU	CD-OE2	6.42	1.37	1.25
1	N	77	SER	CB-OG	6.32	1.54	1.42
1	F	50	VAL	CA-CB	6.26	1.62	1.54
1	E	171	VAL	CA-CB	-5.96	1.47	1.54
1	A	161	ILE	CA-CB	5.88	1.60	1.53
1	G	212	TYR	C-O	5.80	1.30	1.24
1	Q	38	GLU	CD-OE2	5.74	1.36	1.25
1	C	41	GLN	CD-NE2	5.72	1.45	1.33
1	D	153	ASN	C-O	-5.64	1.17	1.24
1	I	27	THR	CA-CB	5.52	1.62	1.53
1	O	28	ASN	CA-C	5.43	1.58	1.52
1	G	81	VAL	CA-CB	5.40	1.61	1.54
1	D	150	ILE	CA-CB	5.39	1.61	1.54
1	I	33	SER	C-O	5.39	1.34	1.23
1	Q	38	GLU	CD-OE1	5.34	1.35	1.25
1	N	105	ASN	CG-ND2	-5.30	1.22	1.33
1	C	37	ALA	C-N	5.28	1.40	1.33
1	E	17	VAL	CA-CB	5.25	1.61	1.54
1	I	115	ALA	CA-CB	-5.20	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	41	GLN	CD-OE1	5.11	1.33	1.23
1	E	42	ARG	N-CA	-5.03	1.39	1.46

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	21	ILE	CB-CA-C	-11.03	101.36	111.06
1	G	214	GLU	CA-C-O	-10.99	102.11	120.80
1	J	28	ASN	N-CA-C	9.50	116.52	108.07
1	N	41	GLN	CA-C-N	-8.49	108.90	120.44
1	N	41	GLN	C-N-CA	-8.49	108.90	120.44
1	K	21	ILE	CB-CA-C	-8.29	103.77	111.06
1	N	39	PHE	CA-C-O	7.25	133.13	120.80
1	S	126	VAL	CB-CA-C	-6.94	100.13	110.82
1	R	179	VAL	CB-CA-C	-6.90	100.94	111.08
1	N	41	GLN	CA-C-O	6.83	128.01	120.63
1	S	50	VAL	CB-CA-C	-6.70	101.24	112.16
1	H	50	VAL	CB-CA-C	-6.47	101.62	112.16
1	N	126	VAL	CB-CA-C	-6.35	101.05	110.82
1	N	41	GLN	O-C-N	6.33	128.82	122.12
1	O	50	VAL	CB-CA-C	-6.25	101.97	112.16
1	B	30	THR	N-CA-C	-6.23	104.18	110.97
1	A	126	VAL	CB-CA-C	-6.12	101.50	110.62
1	C	167	HIS	N-CA-C	6.06	113.67	108.22
1	F	21	ILE	N-CA-CB	-6.04	103.96	112.12
1	B	50	VAL	CB-CA-C	-6.00	102.38	112.16
1	L	21	ILE	N-CA-CB	-5.96	104.08	112.12
1	F	50	VAL	CB-CA-C	-5.90	102.54	112.16
1	A	179	VAL	CB-CA-C	-5.89	102.42	111.08
1	J	126	VAL	CB-CA-C	-5.87	101.87	110.62
1	R	92	LYS	N-CA-CB	5.83	118.69	110.12
1	D	205	PHE	N-CA-C	-5.69	106.94	112.97
1	G	54	VAL	CB-CA-C	5.64	117.35	111.09
1	H	179	VAL	CB-CA-C	-5.62	102.83	111.08
1	Q	0	HIS	N-CA-C	5.61	118.15	110.24
1	L	207	GLU	N-CA-C	-5.56	104.86	111.03
1	O	135	ASP	CB-CA-C	-5.55	100.01	110.67
1	N	0	HIS	N-CA-CB	-5.52	101.11	110.50
1	P	126	VAL	CB-CA-C	-5.48	102.38	110.82
1	J	21	ILE	N-CA-CB	-5.42	104.80	112.12
1	G	182	VAL	N-CA-CB	5.41	118.87	111.41
1	R	179	VAL	N-CA-CB	5.36	121.95	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	206	MET	N-CA-C	-5.27	105.97	112.72
1	J	28	ASN	O-C-N	5.23	126.74	121.56
1	R	116	ILE	N-CA-CB	5.14	118.29	110.58
1	Q	-1	HIS	CA-C-N	5.12	128.12	120.90
1	Q	-1	HIS	C-N-CA	5.12	128.12	120.90
1	N	50	VAL	CB-CA-C	-5.12	103.82	112.16
1	M	81	VAL	CB-CA-C	5.06	118.12	110.63

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	-1	HIS	Peptide
1	N	35	GLU	Sidechain
1	R	37	ALA	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1591	0	1601	34	0
1	B	1584	0	1598	37	0
1	C	1560	0	1561	35	0
1	D	1615	0	1642	31	0
1	E	1674	0	1703	43	0
1	F	1655	0	1680	23	0
1	G	1667	0	1680	30	0
1	H	1550	0	1557	33	0
1	I	1615	0	1623	32	0
1	J	1619	0	1617	52	0
1	K	1651	0	1648	23	0
1	L	1530	0	1521	35	0
1	M	1457	0	1439	38	0
1	N	1475	0	1446	40	0
1	O	1604	0	1613	30	0
1	P	1576	0	1590	25	0
1	Q	1596	0	1594	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	1585	0	1569	35	0
1	S	1533	0	1538	31	0
1	T	1541	0	1521	22	0
2	A	6	0	8	1	0
2	B	6	0	8	1	0
2	C	6	0	8	1	0
2	D	6	0	8	0	0
2	E	6	0	8	0	0
2	F	6	0	8	1	0
2	G	6	0	8	0	0
2	H	6	0	8	2	0
2	I	6	0	8	0	0
2	J	6	0	8	0	0
2	K	10	0	16	0	0
2	L	6	0	8	0	0
2	M	6	0	8	0	0
2	N	6	0	8	0	0
2	O	6	0	8	2	0
2	P	12	0	16	1	0
2	Q	6	0	8	0	0
2	R	6	0	8	0	0
2	S	6	0	8	0	0
2	T	6	0	8	0	0
3	O	5	0	0	0	0
4	A	5	0	0	0	0
4	B	6	0	0	1	0
4	C	7	0	0	0	0
4	D	16	0	0	2	0
4	E	7	0	0	0	0
4	F	5	0	0	0	0
4	G	17	0	0	0	0
4	H	3	0	0	0	0
4	I	4	0	0	0	0
4	J	7	0	0	0	0
4	K	3	0	0	0	0
4	L	1	0	0	0	0
4	M	2	0	0	0	0
4	O	5	0	0	0	0
4	P	3	0	0	0	0
4	Q	7	0	0	0	0
4	R	2	0	0	0	0
4	S	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	T	1	0	0	0	0
All	All	31916	0	31917	573	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (573) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:39:PHE:N	1:N:39:PHE:CA	1.76	1.48
1:G:214:GLU:C	1:G:214:GLU:O	1.67	1.35
1:O:156:PHE:O	2:O:220:GOL:H31	1.63	0.96
1:N:184:MET:HE1	1:N:192:LEU:HD11	1.53	0.87
1:J:128:PRO:HB3	1:J:143:MET:HE1	1.59	0.85
1:L:141:MET:HE1	1:L:144:LEU:HD23	1.57	0.84
1:K:184:MET:HE1	1:K:189:LEU:HB2	1.60	0.83
1:J:28:ASN:CG	1:J:29:PRO:HD2	2.04	0.83
1:B:128:PRO:HB3	1:B:143:MET:HE1	1.60	0.82
1:L:142:ARG:CZ	1:S:142:ARG:HD2	2.10	0.80
1:B:144:LEU:HD13	1:B:177:MET:HE1	1.64	0.80
1:K:184:MET:CE	1:K:189:LEU:HB2	2.12	0.79
1:K:86:MET:HE2	1:K:106:VAL:HG11	1.65	0.79
1:J:28:ASN:CB	1:J:29:PRO:HD2	2.11	0.79
1:J:31:LEU:O	1:J:35:GLU:HG2	1.82	0.79
1:G:130:VAL:HG11	1:G:141:MET:HE2	1.65	0.78
1:D:7:THR:HG22	4:D:226:HOH:O	1.82	0.77
1:A:28:ASN:HB2	1:A:29:PRO:HD2	1.65	0.77
1:K:184:MET:HE1	1:K:189:LEU:CB	2.14	0.77
1:J:28:ASN:OD1	1:J:29:PRO:HD2	1.86	0.75
1:S:184:MET:HE2	1:S:189:LEU:HA	1.66	0.75
1:Q:120:LYS:NZ	1:R:23:ASP:OD2	2.20	0.74
1:D:74:ALA:HA	1:D:80:VAL:HG11	1.68	0.74
1:D:130:VAL:HG11	1:D:141:MET:HE2	1.68	0.74
1:G:40:LYS:HG2	1:G:76:ILE:HD11	1.70	0.74
1:S:184:MET:HE1	1:S:192:LEU:HD11	1.69	0.74
1:J:128:PRO:HB3	1:J:143:MET:CE	2.18	0.73
1:A:174:ALA:HB1	1:A:179:VAL:HG21	1.70	0.73
1:F:27:THR:O	1:F:83:LYS:NZ	2.20	0.73
1:N:27:THR:O	1:N:83:LYS:NZ	2.22	0.73
1:K:28:ASN:ND2	1:K:31:LEU:H	1.87	0.72
1:B:70:ALA:HB1	1:B:82:ILE:HD13	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:THR:O	1:E:83:LYS:NZ	2.22	0.72
1:E:184:MET:HE1	1:E:192:LEU:CD1	2.20	0.71
1:G:27:THR:HG22	1:G:55:SER:O	1.90	0.71
1:K:86:MET:HE1	1:K:91:ILE:HD11	1.73	0.71
1:N:144:LEU:HD21	1:N:179:VAL:HG21	1.73	0.71
1:J:8:ALA:HB3	1:J:35:GLU:HG3	1.73	0.70
1:O:184:MET:HE3	1:O:188:VAL:HG12	1.73	0.70
1:P:40:LYS:O	1:P:41:GLN:HB2	1.90	0.70
1:S:77:SER:O	1:S:80:VAL:HG12	1.90	0.70
1:K:28:ASN:HD22	1:K:28:ASN:C	1.98	0.70
1:N:120:LYS:NZ	1:O:23:ASP:OD2	2.24	0.70
1:C:184:MET:HE1	1:C:189:LEU:HA	1.73	0.70
1:H:203:GLU:C	1:H:205:PHE:H	2.00	0.70
1:D:172:VAL:HG21	1:H:137:SER:HB2	1.72	0.70
1:K:184:MET:HE1	1:K:189:LEU:CA	2.22	0.69
1:J:86:MET:HE1	1:J:118:ALA:HB2	1.75	0.69
1:R:120:LYS:NZ	1:S:23:ASP:OD2	2.25	0.69
1:B:184:MET:HE2	1:B:189:LEU:HA	1.74	0.69
1:A:27:THR:O	1:A:83:LYS:NZ	2.22	0.69
1:D:7:THR:HG21	1:D:12:GLU:OE1	1.92	0.69
1:N:86:MET:HE2	1:N:106:VAL:HG11	1.74	0.69
1:N:184:MET:HE2	1:N:189:LEU:HA	1.75	0.68
1:E:133:MET:HG3	1:E:143:MET:HE2	1.76	0.68
1:H:13:ILE:O	1:H:17:VAL:HG23	1.94	0.68
1:A:117:LEU:HD22	1:B:21:ILE:HD12	1.76	0.68
1:J:86:MET:HE2	1:J:106:VAL:HG11	1.73	0.68
1:H:86:MET:HE2	1:H:106:VAL:HG11	1.74	0.68
1:D:27:THR:O	1:D:83:LYS:NZ	2.22	0.68
1:G:27:THR:O	1:G:83:LYS:NZ	2.26	0.67
1:H:202:ILE:O	1:H:205:PHE:HB3	1.95	0.67
1:E:184:MET:CE	1:E:189:LEU:HA	2.24	0.67
1:K:135:ASP:OD2	1:K:166:ARG:NH2	2.28	0.67
1:H:203:GLU:O	1:H:205:PHE:N	2.26	0.67
1:O:156:PHE:O	2:O:220:GOL:C3	2.39	0.66
1:A:120:LYS:NZ	1:B:23:ASP:OD2	2.26	0.66
1:N:77:SER:O	1:N:80:VAL:HG12	1.94	0.66
1:Q:135:ASP:OD2	1:Q:166:ARG:NH2	2.28	0.66
1:O:137:SER:HB3	1:Q:172:VAL:HG21	1.76	0.66
1:C:144:LEU:HG	1:C:177:MET:HE1	1.77	0.66
1:M:184:MET:HE2	1:M:189:LEU:N	2.11	0.66
1:H:60:SER:HB2	1:H:69:GLU:OE2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:184:MET:HE2	1:S:189:LEU:CA	2.26	0.65
1:A:73:LEU:HD23	1:A:76:ILE:HD11	1.78	0.65
1:J:143:MET:HE3	1:J:147:ILE:HD12	1.78	0.65
1:E:184:MET:HE1	1:E:192:LEU:HD11	1.78	0.65
1:H:27:THR:O	1:H:83:LYS:NZ	2.25	0.65
1:I:95:LYS:HG3	1:J:20:GLY:HA3	1.77	0.65
1:L:110:PHE:CE1	1:L:129:PHE:HB2	2.33	0.64
1:M:144:LEU:HD21	1:M:179:VAL:HG21	1.79	0.64
1:G:86:MET:HE2	1:G:106:VAL:HG11	1.78	0.64
1:O:28:ASN:CG	1:O:29:PRO:HD2	2.23	0.64
1:S:120:LYS:HE3	1:T:1:MET:O	1.97	0.64
1:J:144:LEU:HD21	1:J:179:VAL:HG21	1.81	0.63
1:O:144:LEU:HG	1:O:177:MET:HE1	1.80	0.63
1:A:144:LEU:HG	1:A:177:MET:HE1	1.80	0.63
1:T:184:MET:HE1	1:T:192:LEU:HD11	1.81	0.63
1:N:39:PHE:N	1:N:39:PHE:C	2.56	0.63
1:F:86:MET:HE2	1:F:106:VAL:HG11	1.79	0.63
1:N:184:MET:HE2	1:N:189:LEU:CA	2.29	0.62
1:J:184:MET:HE2	1:J:189:LEU:HB2	1.82	0.62
1:E:21:ILE:HD12	1:E:189:LEU:HD11	1.82	0.62
1:P:120:LYS:NZ	1:Q:23:ASP:OD2	2.27	0.62
1:C:120:LYS:NZ	1:D:23:ASP:OD2	2.25	0.62
1:T:25:VAL:CG2	1:T:50:VAL:HG21	2.30	0.62
1:A:28:ASN:CB	1:A:29:PRO:HD2	2.30	0.61
1:E:137:SER:HB3	1:G:172:VAL:HG21	1.82	0.61
1:M:12:GLU:OE1	1:M:186:PHE:HB2	2.00	0.61
1:P:1:MET:O	1:T:120:LYS:NZ	2.29	0.61
1:A:26:THR:HG23	1:A:83:LYS:NZ	2.16	0.61
1:G:29:PRO:HD3	1:G:57:GLU:CD	2.26	0.61
1:N:184:MET:HE3	1:N:188:VAL:HG12	1.82	0.61
1:F:2:LYS:HB2	1:F:181:ILE:HG12	1.81	0.60
1:A:1:MET:HE1	1:E:116:ILE:HD13	1.81	0.60
1:B:184:MET:HE1	1:B:192:LEU:CD2	2.31	0.60
1:A:174:ALA:HB1	1:A:179:VAL:CG2	2.31	0.60
1:G:95:LYS:NZ	1:H:17:VAL:O	2.31	0.60
1:S:184:MET:HE1	1:S:192:LEU:CD1	2.31	0.60
1:A:189:LEU:HA	1:A:192:LEU:HD22	1.84	0.60
1:O:184:MET:HE3	1:O:188:VAL:CG1	2.32	0.60
1:B:116:ILE:HD11	1:C:3:ILE:HD11	1.84	0.59
1:C:90:GLY:O	1:C:94:VAL:HG23	2.02	0.59
1:R:39:PHE:O	1:R:43:VAL:HG23	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:184:MET:HE2	1:I:189:LEU:N	2.16	0.59
1:J:9:ASN:HB3	1:J:12:GLU:HG2	1.83	0.59
1:C:184:MET:HE1	1:C:189:LEU:CA	2.31	0.59
1:M:86:MET:HE2	1:M:106:VAL:HG11	1.85	0.59
1:E:1:MET:HE3	1:E:182:VAL:HG12	1.83	0.59
1:M:184:MET:HE2	1:M:189:LEU:CA	2.32	0.59
1:L:77:SER:O	1:L:80:VAL:HG12	2.02	0.59
1:T:184:MET:CE	1:T:188:VAL:HG12	2.33	0.59
1:B:143:MET:HE3	1:B:147:ILE:HD11	1.84	0.59
1:I:57:GLU:HA	1:I:83:LYS:HB2	1.85	0.59
1:J:27:THR:HG23	1:J:32:ILE:HD11	1.83	0.59
1:N:0:HIS:N	1:N:0:HIS:CD2	2.66	0.59
1:Q:-1:HIS:CG	1:Q:0:HIS:H	2.20	0.59
1:Q:169:MET:O	1:Q:173:GLU:HG3	2.02	0.59
1:A:26:THR:HG23	1:A:83:LYS:HZ2	1.68	0.59
1:D:137:SER:HB2	1:H:172:VAL:HG21	1.85	0.59
1:N:184:MET:HE1	1:N:192:LEU:CD1	2.28	0.58
1:P:74:ALA:HA	1:P:80:VAL:CG1	2.31	0.58
1:B:116:ILE:HD13	1:C:1:MET:HE2	1.84	0.58
1:H:152:ASN:OD1	2:H:219:GOL:H31	2.03	0.58
1:M:107:THR:HG23	1:M:108:LEU:HG	1.85	0.58
1:R:28:ASN:OD1	1:R:30:THR:OG1	2.20	0.58
1:D:117:LEU:HD22	1:E:21:ILE:HD13	1.85	0.58
1:M:184:MET:HE3	1:M:188:VAL:HB	1.83	0.58
1:F:151:TYR:HB3	2:F:219:GOL:H31	1.85	0.58
1:P:1:MET:HE2	1:P:182:VAL:HG23	1.86	0.58
1:E:184:MET:HE2	1:E:189:LEU:HB2	1.86	0.58
1:N:141:MET:HE2	1:N:141:MET:HA	1.86	0.58
1:A:73:LEU:O	1:A:76:ILE:HG13	2.03	0.57
1:F:116:ILE:CG2	1:F:150:ILE:HG21	2.33	0.57
1:K:28:ASN:HD21	1:K:31:LEU:H	1.51	0.57
1:J:19:TRP:HB3	1:J:21:ILE:HD12	1.86	0.57
1:N:74:ALA:HA	1:N:80:VAL:HG11	1.85	0.57
1:C:151:TYR:HB3	2:C:219:GOL:H31	1.85	0.57
1:P:74:ALA:HA	1:P:80:VAL:HG11	1.86	0.57
1:J:28:ASN:CB	1:J:29:PRO:CD	2.81	0.57
1:B:142:ARG:HD3	1:I:142:ARG:CZ	2.35	0.57
1:J:184:MET:HE1	1:J:189:LEU:HA	1.85	0.57
1:L:27:THR:O	1:L:83:LYS:NZ	2.23	0.57
1:L:74:ALA:HA	1:L:80:VAL:HG11	1.87	0.57
1:R:26:THR:HB	1:R:83:LYS:HZ1	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ASN:HB3	1:A:12:GLU:HG2	1.87	0.57
1:A:137:SER:HB2	1:F:172:VAL:HG21	1.87	0.57
1:B:142:ARG:HD3	1:I:142:ARG:NE	2.19	0.57
1:C:120:LYS:HE3	1:D:1:MET:O	2.04	0.57
1:J:184:MET:CE	1:J:189:LEU:HA	2.35	0.57
1:L:95:LYS:HG3	1:M:20:GLY:HA3	1.87	0.57
1:L:120:LYS:HE3	1:M:1:MET:O	2.03	0.57
1:M:90:GLY:O	1:M:94:VAL:HG23	2.04	0.57
1:O:9:ASN:HB3	1:O:12:GLU:CG	2.34	0.57
1:A:174:ALA:O	1:A:179:VAL:HG23	2.05	0.57
1:C:40:LYS:HG2	1:C:76:ILE:HD11	1.86	0.57
1:H:203:GLU:C	1:H:205:PHE:N	2.62	0.57
1:H:184:MET:HE1	1:H:192:LEU:CD1	2.35	0.56
1:N:172:VAL:HG21	1:R:137:SER:HB3	1.87	0.56
1:E:86:MET:HE2	1:E:106:VAL:HG11	1.86	0.56
1:H:184:MET:HE1	1:H:192:LEU:HD11	1.88	0.56
1:N:0:HIS:CD2	1:N:0:HIS:H3	2.23	0.56
1:P:51:LYS:O	2:P:220:GOL:H11	2.05	0.56
1:J:86:MET:HE2	1:J:106:VAL:CG1	2.35	0.56
1:A:12:GLU:HB2	1:A:186:PHE:CD1	2.41	0.56
1:L:61:LEU:O	1:L:66:MET:HE2	2.06	0.56
1:N:137:SER:HB2	1:R:172:VAL:HG21	1.88	0.56
1:C:5:LEU:HB3	1:C:7:THR:HG22	1.88	0.56
1:R:116:ILE:HD11	1:S:3:ILE:HD11	1.87	0.56
1:M:172:VAL:HG21	1:S:137:SER:HB3	1.87	0.56
1:O:172:VAL:HG21	1:Q:137:SER:OG	2.06	0.55
1:C:58:VAL:HG21	1:C:66:MET:HG2	1.87	0.55
1:F:116:ILE:HG21	1:F:150:ILE:HG21	1.88	0.55
1:F:144:LEU:HD21	1:F:179:VAL:HG21	1.87	0.55
1:R:25:VAL:HG23	1:R:50:VAL:HG21	1.88	0.55
1:A:110:PHE:CE1	1:A:129:PHE:HB2	2.41	0.55
1:E:46:ILE:O	1:E:50:VAL:HG12	2.07	0.55
1:R:19:TRP:HB3	1:R:21:ILE:HD12	1.87	0.55
1:E:9:ASN:HB3	1:E:12:GLU:HG2	1.88	0.55
1:E:191:LYS:NZ	1:G:135:ASP:OD2	2.39	0.54
1:B:184:MET:HE1	1:B:192:LEU:HD22	1.88	0.54
1:E:66:MET:HE1	1:E:90:GLY:HA2	1.88	0.54
1:M:13:ILE:O	1:M:17:VAL:HG23	2.07	0.54
1:D:39:PHE:O	1:D:43:VAL:HG23	2.07	0.54
1:G:214:GLU:O	1:G:214:GLU:CA	2.54	0.54
1:M:166:ARG:H	1:M:170:HIS:HD2	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:26:THR:HG22	1:N:55:SER:OG	2.07	0.54
1:R:0:HIS:ND1	1:R:0:HIS:N	2.54	0.54
1:M:91:ILE:HD12	1:N:193:PHE:CE2	2.42	0.54
1:H:184:MET:CE	1:H:189:LEU:HA	2.37	0.54
1:N:117:LEU:HD22	1:O:21:ILE:CD1	2.38	0.54
1:R:26:THR:HB	1:R:83:LYS:NZ	2.23	0.54
1:E:2:LYS:HB2	1:E:181:ILE:HG23	1.90	0.54
1:A:139:ASP:HB3	1:J:142:ARG:NH2	2.23	0.53
1:I:61:LEU:O	1:I:66:MET:HE2	2.08	0.53
1:C:30:THR:O	1:C:34:LYS:HB2	2.08	0.53
1:C:143:MET:CE	1:C:147:ILE:HD12	2.37	0.53
1:D:74:ALA:HA	1:D:80:VAL:CG1	2.36	0.53
1:J:12:GLU:HB2	1:J:186:PHE:CD1	2.43	0.53
1:E:40:LYS:HB3	1:E:76:ILE:HD11	1.90	0.53
1:J:184:MET:CE	1:J:189:LEU:CA	2.87	0.53
1:L:28:ASN:ND2	1:L:30:THR:OG1	2.41	0.53
1:M:157:GLU:CD	1:M:157:GLU:H	2.17	0.53
1:E:40:LYS:O	1:E:41:GLN:CB	2.57	0.53
1:H:39:PHE:O	1:H:43:VAL:HG23	2.08	0.53
1:K:184:MET:HE1	1:K:189:LEU:HA	1.91	0.53
1:E:184:MET:CE	1:E:189:LEU:CA	2.87	0.53
1:S:91:ILE:HG23	1:S:121:ALA:HB2	1.90	0.53
1:M:120:LYS:NZ	1:N:3:ILE:HD12	2.24	0.53
1:R:143:MET:HG3	1:R:144:LEU:N	2.23	0.53
1:G:46:ILE:O	1:G:50:VAL:HG12	2.09	0.53
1:K:120:LYS:NZ	1:L:23:ASP:OD2	2.29	0.53
1:A:173:GLU:O	1:A:177:MET:HG3	2.08	0.52
1:B:152:ASN:OD1	2:B:219:GOL:O3	2.27	0.52
1:J:28:ASN:O	1:J:32:ILE:N	2.38	0.52
1:B:142:ARG:HD3	1:I:142:ARG:HD2	1.90	0.52
1:I:120:LYS:HE3	1:J:1:MET:O	2.09	0.52
1:J:9:ASN:HB3	1:J:12:GLU:CG	2.38	0.52
1:L:74:ALA:HA	1:L:80:VAL:CG1	2.39	0.52
1:M:29:PRO:HD2	1:M:57:GLU:OE2	2.09	0.52
1:M:130:VAL:HG11	1:M:141:MET:HE2	1.91	0.52
1:H:46:ILE:HG22	1:H:54:VAL:HG21	1.91	0.52
1:A:137:SER:OG	1:J:111:SER:HB2	2.10	0.52
1:D:88:PRO:HA	1:E:193:PHE:CE2	2.44	0.52
1:D:142:ARG:HG2	1:G:142:ARG:CZ	2.40	0.52
1:D:149:GLU:HG2	1:E:176:LEU:HD23	1.92	0.52
1:F:216:LEU:HD12	1:F:216:LEU:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:86:MET:CE	1:J:106:VAL:HG11	2.40	0.52
1:F:205:PHE:CD1	1:J:29:PRO:HG2	2.45	0.52
1:F:87:THR:HB	1:F:88:PRO:HD2	1.92	0.52
1:G:120:LYS:HE3	1:H:1:MET:O	2.10	0.52
1:J:13:ILE:HG21	1:J:50:VAL:HG22	1.92	0.52
1:E:184:MET:HE1	1:E:192:LEU:HD12	1.91	0.52
1:L:184:MET:HE2	1:L:189:LEU:HB2	1.91	0.52
1:C:143:MET:CE	1:C:147:ILE:CD1	2.88	0.51
1:M:86:MET:SD	1:M:91:ILE:HD11	2.51	0.51
1:P:120:LYS:NZ	1:Q:1:MET:O	2.43	0.51
1:Q:133:MET:HG3	1:Q:143:MET:CE	2.39	0.51
1:B:142:ARG:HD3	1:I:142:ARG:CD	2.39	0.51
1:O:184:MET:CE	1:O:188:VAL:HG12	2.40	0.51
1:J:132:ARG:O	1:J:136:LEU:HD13	2.11	0.51
1:M:120:LYS:HZ1	1:N:3:ILE:HD12	1.76	0.51
1:T:130:VAL:HG11	1:T:141:MET:HE2	1.92	0.51
1:J:32:ILE:HD13	1:J:39:PHE:CD1	2.45	0.51
1:C:174:ALA:HA	1:C:177:MET:HE2	1.92	0.51
1:D:130:VAL:CG1	1:D:141:MET:HE2	2.40	0.51
1:G:5:LEU:HB3	1:G:7:THR:HG22	1.92	0.51
1:G:212:TYR:O	1:G:213:LEU:C	2.53	0.51
1:J:27:THR:CG2	1:J:32:ILE:HD11	2.40	0.51
1:N:133:MET:HG3	1:N:143:MET:HE2	1.92	0.51
1:Q:162:ALA:HB1	1:Q:165:ILE:HD11	1.92	0.51
1:T:184:MET:HE2	1:T:189:LEU:N	2.26	0.51
1:G:174:ALA:HB1	1:G:179:VAL:HG11	1.93	0.51
1:G:211:LYS:O	1:G:214:GLU:HB2	2.11	0.51
1:I:21:ILE:HG22	1:I:21:ILE:O	2.11	0.51
1:S:28:ASN:OD1	1:S:30:THR:OG1	2.23	0.51
1:S:46:ILE:O	1:S:50:VAL:HG23	2.10	0.51
1:A:73:LEU:CD2	1:A:76:ILE:HD11	2.40	0.50
1:C:86:MET:HE3	1:C:114:GLN:HB3	1.92	0.50
1:H:184:MET:HE2	1:H:189:LEU:HD13	1.93	0.50
1:I:120:LYS:NZ	1:J:23:ASP:OD2	2.37	0.50
1:B:184:MET:HE2	1:B:189:LEU:CA	2.41	0.50
1:S:184:MET:CE	1:S:189:LEU:HA	2.37	0.50
1:P:27:THR:O	1:P:83:LYS:NZ	2.26	0.50
1:F:91:ILE:HG21	1:G:21:ILE:CD1	2.41	0.50
1:Q:144:LEU:HD21	1:Q:179:VAL:HG21	1.92	0.50
1:A:5:LEU:HB3	1:A:7:THR:HG22	1.92	0.50
1:I:2:LYS:HB2	1:I:181:ILE:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:8:ALA:HB3	1:L:31:LEU:O	2.11	0.50
1:T:13:ILE:CD1	1:T:46:ILE:HG23	2.42	0.50
1:A:2:LYS:HB2	1:A:181:ILE:HG12	1.93	0.50
1:E:46:ILE:HG22	1:E:54:VAL:HG21	1.93	0.50
1:N:74:ALA:HA	1:N:80:VAL:CG1	2.42	0.50
1:Q:42:ARG:O	1:Q:46:ILE:HG13	2.12	0.50
1:Q:86:MET:HE2	1:Q:106:VAL:HG11	1.92	0.49
1:I:143:MET:CE	1:I:147:ILE:HD12	2.40	0.49
1:I:184:MET:HE2	1:I:189:LEU:CA	2.42	0.49
1:Q:65:GLY:HA2	1:Q:68:ARG:NH2	2.28	0.49
1:T:25:VAL:HG23	1:T:50:VAL:HG21	1.93	0.49
1:B:144:LEU:HD13	1:B:177:MET:CE	2.40	0.49
1:F:46:ILE:O	1:F:50:VAL:HG22	2.12	0.49
1:R:107:THR:HG23	1:R:108:LEU:HG	1.94	0.49
1:T:9:ASN:HB3	1:T:12:GLU:HG2	1.92	0.49
1:M:26:THR:HG22	1:M:83:LYS:HE2	1.94	0.49
1:R:129:PHE:HD2	1:R:132:ARG:HD2	1.78	0.49
1:A:104:THR:O	1:A:124:THR:HB	2.13	0.49
1:N:2:LYS:HB2	1:N:181:ILE:HG12	1.93	0.49
1:P:1:MET:HE2	1:P:182:VAL:CG2	2.41	0.49
1:S:86:MET:HE2	1:S:106:VAL:HG11	1.94	0.49
1:K:13:ILE:O	1:K:17:VAL:HG13	2.13	0.49
1:G:86:MET:HE1	1:G:118:ALA:HB2	1.94	0.49
1:S:120:LYS:NZ	1:T:23:ASP:OD2	2.43	0.49
1:B:32:ILE:HG23	1:B:42:ARG:HG2	1.94	0.49
1:B:184:MET:HE3	1:B:188:VAL:HG12	1.95	0.49
1:G:95:LYS:NZ	1:H:20:GLY:HA2	2.28	0.48
1:L:2:LYS:HB2	1:L:181:ILE:HG12	1.95	0.48
1:B:145:GLY:HA2	1:B:177:MET:HE3	1.95	0.48
1:D:82:ILE:HD13	1:D:102:ILE:CG2	2.43	0.48
1:L:174:ALA:HB1	1:L:179:VAL:HG11	1.96	0.48
1:R:2:LYS:HB2	1:R:181:ILE:HG23	1.94	0.48
1:B:143:MET:CE	1:B:147:ILE:CD1	2.91	0.48
1:C:26:THR:HG22	1:C:55:SER:OG	2.13	0.48
1:E:57:GLU:OE2	1:E:83:LYS:NZ	2.44	0.48
1:J:202:ILE:O	1:J:205:PHE:HB3	2.13	0.48
1:I:184:MET:HE1	1:I:192:LEU:HD11	1.95	0.48
1:L:95:LYS:CG	1:M:20:GLY:HA3	2.44	0.48
1:B:143:MET:HE2	1:B:143:MET:C	2.38	0.48
1:C:86:MET:HE1	1:C:118:ALA:HB2	1.95	0.48
1:O:195:HIS:ND1	1:O:196:PRO:HD2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:11:GLU:O	1:Q:15[B]:LYS:HG3	2.13	0.48
1:B:13:ILE:HG22	1:B:49:LEU:HG	1.96	0.48
1:M:184:MET:CE	1:M:189:LEU:N	2.75	0.48
1:Q:90:GLY:O	1:Q:94:VAL:HG23	2.14	0.48
1:E:184:MET:HE2	1:E:189:LEU:CB	2.43	0.48
1:K:86:MET:HE2	1:K:106:VAL:CG1	2.41	0.48
1:E:57:GLU:CD	1:E:83:LYS:NZ	2.72	0.47
1:H:103:LYS:HG2	1:H:124:THR:HG21	1.96	0.47
1:D:90:GLY:O	1:D:94:VAL:HG23	2.13	0.47
1:E:196:PRO:HB3	1:H:200:LEU:HD11	1.96	0.47
1:J:7:THR:HG21	1:J:12:GLU:OE2	2.14	0.47
1:L:142:ARG:NH1	1:S:142:ARG:HH11	2.12	0.47
1:E:28:ASN:HA	1:E:57:GLU:OE2	2.15	0.47
1:L:141:MET:CE	1:L:144:LEU:HD23	2.38	0.47
1:S:143:MET:HG3	1:S:144:LEU:N	2.30	0.47
1:C:120:LYS:NZ	1:D:21:ILE:O	2.47	0.47
1:A:120:LYS:NZ	1:B:1:MET:O	2.47	0.47
1:B:25:VAL:HG23	1:B:50:VAL:HG11	1.97	0.47
1:P:95:LYS:HG3	1:Q:20:GLY:HA3	1.97	0.47
1:C:9:ASN:HB3	1:C:12:GLU:HG2	1.97	0.47
1:E:130:VAL:HG11	1:E:141:MET:CE	2.43	0.47
1:F:20:GLY:HA3	1:J:95:LYS:HD2	1.97	0.47
1:J:27:THR:HB	1:J:55:SER:O	2.14	0.47
1:A:165:ILE:HG12	1:A:182:VAL:HG23	1.97	0.47
1:D:19:TRP:HB3	1:D:21:ILE:HD12	1.97	0.47
1:F:113:ALA:HB1	1:G:192:LEU:HD22	1.97	0.47
1:N:184:MET:HE2	1:N:189:LEU:N	2.30	0.47
1:S:117:LEU:HD22	1:T:21:ILE:HD13	1.97	0.47
1:D:7:THR:CG2	4:D:226:HOH:O	2.54	0.47
1:G:2:LYS:HB2	1:G:181:ILE:HG12	1.96	0.47
1:L:29:PRO:HD3	1:L:57:GLU:HG3	1.96	0.47
1:Q:141:MET:O	1:Q:177:MET:HE1	2.15	0.47
1:J:2:LYS:HB2	1:J:181:ILE:HG12	1.97	0.47
1:B:142:ARG:O	1:B:146:GLU:HG3	2.15	0.47
1:B:188:VAL:O	1:B:192:LEU:HD13	2.14	0.47
1:O:31:LEU:H	1:O:31:LEU:HD12	1.80	0.47
1:F:63:TYR:HA	1:F:66:MET:HE3	1.98	0.46
1:K:28:ASN:ND2	1:K:28:ASN:C	2.71	0.46
1:A:120:LYS:NZ	1:B:2:LYS:HA	2.30	0.46
1:L:184:MET:HE2	1:L:189:LEU:CA	2.45	0.46
1:Q:213:LEU:N	1:Q:213:LEU:HD12	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:154:TYR:OH	1:M:179:VAL:O	2.27	0.46
1:R:72:GLU:O	1:R:75:GLN:OE1	2.33	0.46
1:C:203:GLU:O	1:C:207:GLU:HB2	2.16	0.46
1:L:143:MET:HG3	1:L:144:LEU:N	2.30	0.46
1:I:184:MET:HE3	1:I:188:VAL:HG12	1.98	0.46
1:K:19:TRP:HB3	1:K:21:ILE:HD12	1.98	0.46
1:L:143:MET:HE2	1:L:147:ILE:HD11	1.98	0.46
1:L:142:ARG:NE	1:S:142:ARG:HD2	2.30	0.46
1:N:7:THR:CA	1:N:31:LEU:HD13	2.46	0.46
1:F:182:VAL:HG22	1:F:184:MET:HE2	1.98	0.46
1:K:131:GLY:O	1:K:135:ASP:OD2	2.34	0.46
1:P:144:LEU:HD21	1:P:179:VAL:HG21	1.98	0.46
1:R:86:MET:HE2	1:R:106:VAL:HG11	1.98	0.46
1:O:188:VAL:O	1:O:192:LEU:HD13	2.15	0.46
1:R:141:MET:HE2	1:R:173:GLU:HB3	1.98	0.46
1:E:32:ILE:HG23	1:E:37:ALA:HB3	1.96	0.45
1:G:78:GLU:O	1:G:103:LYS:NZ	2.48	0.45
1:H:152:ASN:OD1	2:H:219:GOL:C3	2.64	0.45
1:E:205:PHE:CD1	1:E:205:PHE:C	2.94	0.45
1:R:25:VAL:CG2	1:R:50:VAL:HG21	2.46	0.45
1:T:13:ILE:HD12	1:T:50:VAL:CG2	2.46	0.45
1:N:5:LEU:HB3	1:N:7:THR:HG22	1.98	0.45
1:J:46:ILE:O	1:J:50:VAL:HG23	2.17	0.45
1:Q:188:VAL:O	1:Q:192:LEU:HD13	2.16	0.45
1:I:28:ASN:ND2	1:I:30:THR:OG1	2.35	0.45
1:T:212:TYR:CD1	1:T:212:TYR:C	2.94	0.45
1:F:140:GLY:O	1:F:143:MET:HG3	2.16	0.45
1:J:6:ASP:OD1	1:J:31:LEU:HD11	2.15	0.45
1:J:55:SER:HB3	1:J:83:LYS:HG3	1.99	0.45
1:I:210:LYS:HA	1:I:213:LEU:HD12	1.99	0.45
1:K:110:PHE:CE2	1:K:129:PHE:HB2	2.52	0.45
1:N:134:ASP:OD1	1:N:140:GLY:N	2.46	0.45
1:P:143:MET:HE3	1:P:143:MET:HB2	1.79	0.45
1:Q:212:TYR:O	1:Q:212:TYR:CG	2.69	0.45
1:I:8:ALA:HB3	1:I:31:LEU:O	2.17	0.45
1:M:166:ARG:H	1:M:170:HIS:CD2	2.33	0.45
1:R:184:MET:HE1	1:R:192:LEU:HD22	1.99	0.45
1:T:165:ILE:HD12	1:T:170:HIS:HB3	1.98	0.45
1:M:4:PHE:CZ	1:M:53:PRO:HG2	2.52	0.45
1:N:184:MET:HE3	1:N:188:VAL:CG1	2.47	0.45
1:G:120:LYS:NZ	1:H:23:ASP:OD2	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:31:LEU:O	1:N:32:ILE:C	2.60	0.44
1:O:144:LEU:HD21	1:O:179:VAL:HG21	1.99	0.44
1:R:184:MET:HE2	1:R:189:LEU:N	2.32	0.44
1:I:63:TYR:O	1:I:67:VAL:HG23	2.17	0.44
1:J:2:LYS:HA	1:J:23:ASP:OD2	2.17	0.44
1:J:31:LEU:O	1:J:35:GLU:CG	2.58	0.44
1:L:39:PHE:O	1:L:40:LYS:C	2.60	0.44
1:P:3:ILE:HG23	1:P:184:MET:HE3	1.99	0.44
1:R:174:ALA:HB1	1:R:179:VAL:CG2	2.48	0.44
1:S:12:GLU:HB2	1:S:186:PHE:CD1	2.52	0.44
1:F:10:LEU:HD22	1:F:49:LEU:HD12	1.99	0.44
1:Q:2:LYS:HB2	1:Q:181:ILE:HG23	1.99	0.44
1:H:39:PHE:HB2	1:I:212:TYR:OH	2.17	0.44
1:I:147:ILE:HG22	1:I:160:ILE:HD13	2.00	0.44
1:O:148:VAL:HG21	1:O:179:VAL:HG22	2.00	0.44
1:F:21:ILE:CD1	1:J:91:ILE:HG21	2.47	0.44
1:B:167:HIS:CD2	4:B:220:HOH:O	2.70	0.44
1:O:7:THR:HG23	1:O:13:ILE:HD11	2.00	0.44
1:O:184:MET:HE2	1:O:189:LEU:HA	2.00	0.44
1:Q:82:ILE:HD13	1:Q:102:ILE:CG2	2.47	0.44
1:R:214:GLU:O	1:R:215:ASN:C	2.60	0.44
1:J:184:MET:HE2	1:J:189:LEU:CB	2.46	0.44
1:L:184:MET:CE	1:L:189:LEU:HA	2.48	0.44
1:M:154:TYR:OH	1:N:179:VAL:O	2.27	0.44
1:Q:19:TRP:HB2	1:Q:21:ILE:HG12	1.98	0.44
1:R:143:MET:HE3	1:R:143:MET:HB2	1.82	0.44
1:C:174:ALA:HB1	1:C:179:VAL:HG11	2.00	0.44
1:D:2:LYS:HB2	1:D:181:ILE:HG12	2.00	0.44
1:J:125:TYR:CD2	1:J:161:ILE:HD11	2.52	0.44
1:P:3:ILE:HD12	1:T:120:LYS:HD3	2.00	0.44
1:E:86:MET:HE2	1:E:106:VAL:CG1	2.47	0.43
1:R:29:PRO:O	1:R:30:THR:C	2.61	0.43
1:B:143:MET:HE3	1:B:147:ILE:CD1	2.47	0.43
1:H:184:MET:HE3	1:H:189:LEU:HA	1.98	0.43
1:I:10:LEU:HD23	1:I:13:ILE:HD12	2.00	0.43
1:L:0:HIS:HB2	1:L:2:LYS:HZ3	1.81	0.43
1:L:88:PRO:HA	1:M:193:PHE:CE2	2.53	0.43
1:S:184:MET:HE3	1:S:188:VAL:HG12	2.00	0.43
1:C:27:THR:O	1:C:83:LYS:HE2	2.17	0.43
1:G:143:MET:HE1	1:G:147:ILE:HD11	2.00	0.43
1:H:149:GLU:HG2	1:I:176:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ILE:HD12	1:B:102:ILE:CG2	2.48	0.43
1:H:57:GLU:HA	1:H:83:LYS:HB2	2.01	0.43
1:I:63:TYR:CE1	1:I:67:VAL:HG21	2.54	0.43
1:L:64:GLU:CD	1:L:64:GLU:H	2.27	0.43
1:N:87:THR:HB	1:N:88:PRO:HD2	2.00	0.43
1:D:2:LYS:HB2	1:D:181:ILE:HG23	1.99	0.43
1:J:100:GLU:HG3	1:J:102:ILE:HD12	1.99	0.43
1:N:113:ALA:HB1	1:O:192:LEU:HG	1.99	0.43
1:P:1:MET:HE3	1:P:175:ALA:HA	1.99	0.43
1:Q:202:ILE:O	1:Q:206:MET:HB2	2.18	0.43
1:R:9:ASN:OD1	1:R:9:ASN:C	2.62	0.43
1:C:144:LEU:CG	1:C:177:MET:HE1	2.47	0.43
1:F:133:MET:HE3	1:F:133:MET:HB3	1.90	0.43
1:P:120:LYS:NZ	1:Q:2:LYS:HA	2.34	0.43
1:Q:-1:HIS:CG	1:Q:0:HIS:N	2.86	0.43
1:S:4:PHE:CZ	1:S:181:ILE:HD13	2.53	0.43
1:G:212:TYR:O	1:G:214:GLU:C	2.62	0.43
1:J:46:ILE:HG22	1:J:54:VAL:HG21	2.01	0.43
1:S:13:ILE:O	1:S:17:VAL:HG13	2.18	0.43
1:C:188:VAL:O	1:C:192:LEU:HD13	2.19	0.43
1:O:137:SER:HB2	1:P:111:SER:HB2	1.99	0.43
1:E:205:PHE:CD1	1:E:206:MET:N	2.87	0.43
1:J:28:ASN:HB2	1:J:31:LEU:HD12	2.00	0.43
1:M:110:PHE:CE1	1:M:129:PHE:HB2	2.53	0.43
1:O:28:ASN:HB3	1:O:31:LEU:CD1	2.49	0.42
1:E:28:ASN:HB2	1:E:29:PRO:HD2	2.00	0.42
1:I:90:GLY:O	1:I:94:VAL:HG23	2.18	0.42
1:K:57:GLU:HA	1:K:83:LYS:HB2	2.00	0.42
1:A:141:MET:HE2	1:A:173:GLU:HB3	2.02	0.42
1:C:38:GLU:O	1:C:39:PHE:C	2.62	0.42
1:M:86:MET:HE3	1:M:114:GLN:HB3	2.00	0.42
1:M:157:GLU:CD	1:M:157:GLU:N	2.77	0.42
1:Q:55:SER:HA	1:Q:81:VAL:O	2.19	0.42
1:I:94:VAL:O	1:I:98:SER:OG	2.31	0.42
1:E:184:MET:HE2	1:E:189:LEU:CA	2.49	0.42
1:O:148:VAL:CG2	1:O:179:VAL:HG22	2.49	0.42
1:Q:113:ALA:HB1	1:R:192:LEU:HG	2.01	0.42
1:R:154:TYR:OH	1:S:179:VAL:O	2.31	0.42
1:T:104:THR:O	1:T:124:THR:HB	2.19	0.42
1:D:7:THR:CG2	1:D:12:GLU:OE1	2.64	0.42
1:D:87:THR:HB	1:D:88:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:VAL:HG21	1:G:137:SER:HB3	2.02	0.42
1:N:9:ASN:HB3	1:N:12:GLU:HG2	2.01	0.42
1:S:143:MET:HE3	1:S:143:MET:HB2	1.89	0.42
1:K:20:GLY:HA3	1:O:95:LYS:HG3	2.01	0.42
1:N:86:MET:HE2	1:N:106:VAL:CG1	2.47	0.42
1:N:149:GLU:OE1	1:N:149:GLU:HA	2.19	0.42
1:D:52:GLY:O	1:D:79:TYR:HB3	2.19	0.42
1:E:5:LEU:HB3	1:E:7:THR:HG22	2.00	0.42
1:L:9:ASN:HB3	1:L:12:GLU:HG2	2.02	0.42
1:F:3:ILE:HD12	1:J:120:LYS:HE2	2.02	0.42
1:I:110:PHE:CE1	1:I:129:PHE:HB2	2.55	0.42
1:O:90:GLY:O	1:O:94:VAL:HG23	2.19	0.42
1:R:13:ILE:CG2	1:R:50:VAL:HG22	2.49	0.42
1:C:39:PHE:O	1:C:43:VAL:HG23	2.20	0.42
1:H:86:MET:HE2	1:H:106:VAL:CG1	2.47	0.42
1:M:5:LEU:HB3	1:M:7:THR:HG22	2.02	0.42
1:M:51:LYS:HA	1:M:79:TYR:CE2	2.55	0.42
1:Q:91:ILE:HG21	1:R:21:ILE:HD11	2.02	0.42
1:D:66:MET:HE1	1:D:89:ASP:C	2.45	0.41
1:R:69:GLU:O	1:R:73:LEU:HG	2.19	0.41
1:I:27:THR:O	1:I:83:LYS:NZ	2.43	0.41
1:I:32:ILE:O	1:I:32:ILE:CG2	2.69	0.41
1:M:195:HIS:CG	1:M:196:PRO:HD2	2.55	0.41
1:O:91:ILE:HG23	1:O:121:ALA:HB2	2.02	0.41
1:R:9:ASN:HB3	1:R:12:GLU:HG3	2.02	0.41
1:A:28:ASN:CB	1:A:29:PRO:CD	2.97	0.41
1:C:9:ASN:OD1	1:C:9:ASN:C	2.63	0.41
1:D:130:VAL:HG11	1:D:141:MET:CE	2.43	0.41
1:H:61:LEU:O	1:H:66:MET:HE2	2.20	0.41
1:P:63:TYR:HA	1:P:66:MET:HE3	2.02	0.41
1:H:28:ASN:HB2	1:H:29:PRO:CD	2.50	0.41
1:K:82:ILE:HD13	1:K:102:ILE:CG2	2.50	0.41
1:L:116:ILE:HD11	1:L:150:ILE:HD13	2.02	0.41
1:N:9:ASN:C	1:N:9:ASN:OD1	2.63	0.41
1:P:29:PRO:O	1:P:33:SER:HB2	2.20	0.41
1:S:30:THR:HG23	1:T:208:ASP:HB3	2.00	0.41
1:D:80:VAL:O	1:D:80:VAL:HG13	2.19	0.41
1:S:55:SER:HB3	1:S:83:LYS:HG3	2.02	0.41
1:S:91:ILE:HG21	1:T:21:ILE:HD11	2.03	0.41
1:A:1:MET:HE1	1:E:116:ILE:HG21	2.02	0.41
1:E:130:VAL:HG11	1:E:141:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:111:SER:HA	1:H:143:MET:HE3	2.01	0.41
1:I:128:PRO:HB3	1:I:143:MET:HE1	2.03	0.41
1:M:86:MET:HE1	1:M:118:ALA:HB2	2.03	0.41
1:P:88:PRO:HA	1:Q:193:PHE:CE2	2.55	0.41
1:A:26:THR:CG2	1:A:83:LYS:NZ	2.83	0.41
1:E:86:MET:HE1	1:E:118:ALA:HB2	2.03	0.41
1:R:9:ASN:HB3	1:R:12:GLU:CG	2.51	0.41
1:B:141:MET:HE2	1:B:173:GLU:HB3	2.02	0.41
1:K:165:ILE:HD12	1:K:170:HIS:HB3	2.02	0.41
1:L:9:ASN:OD1	1:L:9:ASN:C	2.64	0.41
1:N:83:LYS:HG2	1:N:107:THR:HG21	2.02	0.41
1:O:110:PHE:CE1	1:O:129:PHE:HB2	2.55	0.41
1:R:86:MET:O	1:S:198:THR:HG21	2.20	0.41
1:B:113:ALA:HB1	1:C:192:LEU:HG	2.03	0.41
1:E:66:MET:HE1	1:E:89:ASP:C	2.46	0.41
1:H:19:TRP:HB3	1:H:21:ILE:HD13	2.03	0.41
1:I:143:MET:HE1	1:I:147:ILE:HD12	2.02	0.41
1:L:-1:HIS:ND1	1:L:2:LYS:HE2	2.35	0.41
1:P:104:THR:O	1:P:124:THR:HB	2.21	0.41
1:P:140:GLY:O	1:P:143:MET:HG3	2.21	0.41
1:B:149:GLU:HG2	1:C:176:LEU:HD23	2.03	0.41
1:C:55:SER:HA	1:C:81:VAL:O	2.21	0.41
1:O:21:ILE:HG21	1:O:21:ILE:HD13	1.86	0.41
1:O:27:THR:O	1:O:83:LYS:HE3	2.21	0.41
1:P:143:MET:HG3	1:P:144:LEU:N	2.35	0.41
1:A:151:TYR:HB3	2:A:219:GOL:H32	2.03	0.40
1:B:52:GLY:O	1:B:54:VAL:HG23	2.21	0.40
1:D:21:ILE:HG21	1:D:21:ILE:HD13	1.88	0.40
1:G:25:VAL:O	1:G:54:VAL:HA	2.20	0.40
1:T:167:HIS:HB2	1:T:168:PRO:CD	2.51	0.40
1:B:90:GLY:O	1:B:94:VAL:HG23	2.22	0.40
1:G:143:MET:HE2	1:G:143:MET:HB2	1.80	0.40
1:J:29:PRO:O	1:J:33:SER:N	2.51	0.40
1:L:63:TYR:HE1	1:L:93:ALA:HA	1.86	0.40
1:C:2:LYS:HB2	1:C:181:ILE:HG12	2.04	0.40
1:C:78:GLU:CD	1:C:78:GLU:H	2.29	0.40
1:D:96:THR:O	1:D:100:GLU:HG3	2.21	0.40
1:M:184:MET:HE3	1:M:188:VAL:CB	2.50	0.40
1:T:174:ALA:HB1	1:T:179:VAL:HG11	2.03	0.40
1:E:167:HIS:O	1:E:170:HIS:HB2	2.21	0.40
1:M:66:MET:HE1	1:M:90:GLY:HA2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:32:ILE:HD13	1:P:39:PHE:HD1	1.86	0.40
1:S:174:ALA:O	1:S:179:VAL:HG23	2.21	0.40
1:T:143:MET:HG3	1:T:144:LEU:N	2.37	0.40
1:C:86:MET:CE	1:C:114:GLN:O	2.69	0.40
1:F:180:ASP:C	1:F:181:ILE:HG13	2.47	0.40
1:M:167:HIS:NE2	1:M:170:HIS:CE1	2.89	0.40
1:O:148:VAL:HG21	1:O:177:MET:CE	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	203/230 (88%)	198 (98%)	5 (2%)	0	100	100
1	B	207/230 (90%)	205 (99%)	2 (1%)	0	100	100
1	C	206/230 (90%)	202 (98%)	3 (2%)	1 (0%)	24	37
1	D	208/230 (90%)	204 (98%)	3 (1%)	1 (0%)	24	37
1	E	214/230 (93%)	210 (98%)	2 (1%)	2 (1%)	14	22
1	F	209/230 (91%)	204 (98%)	5 (2%)	0	100	100
1	G	214/230 (93%)	210 (98%)	3 (1%)	1 (0%)	24	37
1	H	201/230 (87%)	196 (98%)	4 (2%)	1 (0%)	24	37
1	I	207/230 (90%)	202 (98%)	4 (2%)	1 (0%)	24	37
1	J	211/230 (92%)	207 (98%)	4 (2%)	0	100	100
1	K	214/230 (93%)	212 (99%)	2 (1%)	0	100	100
1	L	200/230 (87%)	194 (97%)	5 (2%)	1 (0%)	24	37
1	M	194/230 (84%)	191 (98%)	3 (2%)	0	100	100
1	N	200/230 (87%)	195 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	208/230 (90%)	204 (98%)	4 (2%)	0	100	100
1	P	207/230 (90%)	201 (97%)	5 (2%)	1 (0%)	24	37
1	Q	205/230 (89%)	201 (98%)	3 (2%)	1 (0%)	24	37
1	R	206/230 (90%)	200 (97%)	5 (2%)	1 (0%)	24	37
1	S	203/230 (88%)	199 (98%)	2 (1%)	2 (1%)	12	20
1	T	200/230 (87%)	197 (98%)	2 (1%)	1 (0%)	24	37
All	All	4117/4600 (90%)	4032 (98%)	71 (2%)	14 (0%)	36	50

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	0	HIS
1	P	41	GLN
1	S	38	GLU
1	E	41	GLN
1	H	204	ARG
1	R	213	LEU
1	S	39	PHE
1	C	39	PHE
1	E	39	PHE
1	L	31	LEU
1	D	0	HIS
1	I	213	LEU
1	Q	212	TYR
1	T	29	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	171/196 (87%)	156 (91%)	15 (9%)	9	15
1	B	168/196 (86%)	157 (94%)	11 (6%)	15	27
1	C	165/196 (84%)	151 (92%)	14 (8%)	10	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	175/196 (89%)	165 (94%)	10 (6%)	18	33
1	E	181/196 (92%)	165 (91%)	16 (9%)	9	15
1	F	179/196 (91%)	164 (92%)	15 (8%)	10	17
1	G	179/196 (91%)	167 (93%)	12 (7%)	15	26
1	H	166/196 (85%)	151 (91%)	15 (9%)	9	15
1	I	173/196 (88%)	163 (94%)	10 (6%)	18	32
1	J	172/196 (88%)	156 (91%)	16 (9%)	8	14
1	K	176/196 (90%)	164 (93%)	12 (7%)	14	25
1	L	161/196 (82%)	141 (88%)	20 (12%)	4	6
1	M	152/196 (78%)	140 (92%)	12 (8%)	11	19
1	N	151/196 (77%)	140 (93%)	11 (7%)	13	22
1	O	173/196 (88%)	159 (92%)	14 (8%)	11	18
1	P	167/196 (85%)	155 (93%)	12 (7%)	13	23
1	Q	168/196 (86%)	161 (96%)	7 (4%)	26	45
1	R	167/196 (85%)	152 (91%)	15 (9%)	9	15
1	S	162/196 (83%)	146 (90%)	16 (10%)	7	11
1	T	162/196 (83%)	152 (94%)	10 (6%)	16	29
All	All	3368/3920 (86%)	3105 (92%)	263 (8%)	11	20

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	HIS
1	A	1	MET
1	A	10	LEU
1	A	68	ARG
1	A	76	ILE
1	A	84	ILE
1	A	95	LYS
1	A	126	VAL
1	A	165	ILE
1	A	166	ARG
1	A	179	VAL
1	A	182	VAL
1	A	192	LEU
1	A	210	LYS

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Mol	Chain	Res	Type
1	A	216	LEU
1	B	50	VAL
1	B	75	GLN
1	B	92	LYS
1	B	107	THR
1	B	116	ILE
1	B	143	MET
1	B	144	LEU
1	B	166	ARG
1	B	181	ILE
1	B	184	MET
1	B	206	MET
1	C	17	VAL
1	C	27	THR
1	C	30	THR
1	C	34	LYS
1	C	50	VAL
1	C	64	GLU
1	C	78	GLU
1	C	126	VAL
1	C	143	MET
1	C	166	ARG
1	C	182	VAL
1	C	192	LEU
1	C	205	PHE
1	C	206	MET
1	D	27	THR
1	D	30	THR
1	D	58	VAL
1	D	72	GLU
1	D	83	LYS
1	D	136	LEU
1	D	143	MET
1	D	179	VAL
1	D	204	ARG
1	D	206	MET
1	E	6	ASP
1	E	15	LYS
1	E	27	THR
1	E	30	THR
1	E	40	LYS
1	E	45	GLU

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Mol	Chain	Res	Type
1	E	57	GLU
1	E	72	GLU
1	E	84	ILE
1	E	103	LYS
1	E	120	LYS
1	E	142	ARG
1	E	166	ARG
1	E	184	MET
1	E	205	PHE
1	E	211	LYS
1	F	2	LYS
1	F	11	GLU
1	F	21	ILE
1	F	27	THR
1	F	44	LYS
1	F	49	LEU
1	F	50	VAL
1	F	58	VAL
1	F	76	ILE
1	F	103	LYS
1	F	116	ILE
1	F	143	MET
1	F	166	ARG
1	F	182	VAL
1	F	215	ASN
1	G	21	ILE
1	G	26	THR
1	G	30	THR
1	G	54	VAL
1	G	141	MET
1	G	143	MET
1	G	166	ARG
1	G	182	VAL
1	G	207	GLU
1	G	209	TRP
1	G	210	LYS
1	G	214	GLU
1	H	21	ILE
1	H	27	THR
1	H	30	THR
1	H	33	SER
1	H	42	ARG

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Mol	Chain	Res	Type
1	H	50	VAL
1	H	57	GLU
1	H	58	VAL
1	H	60	SER
1	H	72	GLU
1	H	95	LYS
1	H	111	SER
1	H	143	MET
1	H	166	ARG
1	H	184	MET
1	I	28	ASN
1	I	57	GLU
1	I	58	VAL
1	I	78	GLU
1	I	95	LYS
1	I	98	SER
1	I	103	LYS
1	I	120	LYS
1	I	143	MET
1	I	166	ARG
1	J	6	ASP
1	J	10	LEU
1	J	21	ILE
1	J	27	THR
1	J	42	ARG
1	J	45	GLU
1	J	49	LEU
1	J	50	VAL
1	J	59	VAL
1	J	68	ARG
1	J	75	GLN
1	J	78	GLU
1	J	95	LYS
1	J	126	VAL
1	J	143	MET
1	J	166	ARG
1	K	3	ILE
1	K	12	GLU
1	K	17	VAL
1	K	28	ASN
1	K	30	THR
1	K	58	VAL

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Mol	Chain	Res	Type
1	K	143	MET
1	K	166	ARG
1	K	173	GLU
1	K	179	VAL
1	K	184	MET
1	K	209	TRP
1	L	2	LYS
1	L	15	LYS
1	L	21	ILE
1	L	27	THR
1	L	28	ASN
1	L	30	THR
1	L	32	ILE
1	L	49	LEU
1	L	57	GLU
1	L	58	VAL
1	L	59	VAL
1	L	78	GLU
1	L	107	THR
1	L	124	THR
1	L	126	VAL
1	L	141	MET
1	L	143	MET
1	L	182	VAL
1	L	202	ILE
1	L	208	ASP
1	M	27	THR
1	M	30	THR
1	M	33	SER
1	M	49	LEU
1	M	55	SER
1	M	62	ASP
1	M	68	ARG
1	M	81	VAL
1	M	96	THR
1	M	107	THR
1	M	143	MET
1	M	166	ARG
1	N	0	HIS
1	N	21	ILE
1	N	46	ILE
1	N	50	VAL

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Mol	Chain	Res	Type
1	N	55	SER
1	N	58	VAL
1	N	77	SER
1	N	126	VAL
1	N	141	MET
1	N	166	ARG
1	N	191	LYS
1	O	-1	HIS
1	O	6	ASP
1	O	15	LYS
1	O	21	ILE
1	O	27	THR
1	O	30	THR
1	O	31	LEU
1	O	35	GLU
1	O	50	VAL
1	O	57	GLU
1	O	95	LYS
1	O	120	LYS
1	O	143	MET
1	O	208	ASP
1	P	-1	HIS
1	P	2	LYS
1	P	15	LYS
1	P	27	THR
1	P	33	SER
1	P	41	GLN
1	P	42	ARG
1	P	49	LEU
1	P	126	VAL
1	P	142	ARG
1	P	143	MET
1	P	166	ARG
1	Q	27	THR
1	Q	28	ASN
1	Q	64	GLU
1	Q	72	GLU
1	Q	192	LEU
1	Q	204	ARG
1	Q	209	TRP
1	R	0	HIS
1	R	12	GLU

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Mol	Chain	Res	Type
1	R	27	THR
1	R	59	VAL
1	R	75	GLN
1	R	87	THR
1	R	107	THR
1	R	116	ILE
1	R	142	ARG
1	R	143	MET
1	R	166	ARG
1	R	179	VAL
1	R	182	VAL
1	R	192	LEU
1	R	209	TRP
1	S	2	LYS
1	S	5	LEU
1	S	17	VAL
1	S	27	THR
1	S	30	THR
1	S	50	VAL
1	S	68	ARG
1	S	82	ILE
1	S	120	LYS
1	S	126	VAL
1	S	142	ARG
1	S	143	MET
1	S	166	ARG
1	S	177	MET
1	S	184	MET
1	S	204	ARG
1	T	2	LYS
1	T	27	THR
1	T	60	SER
1	T	62	ASP
1	T	78	GLU
1	T	95	LYS
1	T	103	LYS
1	T	104	THR
1	T	143	MET
1	T	161	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	167	HIS
1	C	167	HIS
1	E	167	HIS
1	H	41	GLN
1	K	28	ASN
1	L	28	ASN
1	M	0	HIS
1	M	167	HIS
1	M	170	HIS
1	N	0	HIS
1	Q	28	ASN
1	T	167	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	O	219	-	4,4,4	0.35	0	6,6,6	0.13	0
2	GOL	J	219	-	5,5,5	0.17	0	5,5,5	0.74	0
2	GOL	A	219	-	5,5,5	0.57	0	5,5,5	1.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	K	219[B]	-	5,5,5	0.42	0	5,5,5	0.29	0
2	GOL	L	219	-	5,5,5	0.31	0	5,5,5	0.29	0
2	GOL	I	219	-	5,5,5	0.23	0	5,5,5	0.67	0
2	GOL	O	220	-	5,5,5	0.43	0	5,5,5	1.59	2 (40%)
2	GOL	C	219	-	5,5,5	0.48	0	5,5,5	1.29	0
2	GOL	K	219[A]	-	5,5,5	0.27	0	5,5,5	0.64	0
2	GOL	F	219	-	5,5,5	0.34	0	5,5,5	0.39	0
2	GOL	D	219	-	5,5,5	0.30	0	5,5,5	1.09	0
2	GOL	H	219	-	5,5,5	0.38	0	5,5,5	1.11	0
2	GOL	P	219	-	5,5,5	0.32	0	5,5,5	0.46	0
2	GOL	N	219	-	5,5,5	0.20	0	5,5,5	0.73	0
2	GOL	M	219	-	5,5,5	0.42	0	5,5,5	0.90	0
2	GOL	S	219	-	5,5,5	0.39	0	5,5,5	0.69	0
2	GOL	P	220	-	5,5,5	0.29	0	5,5,5	0.87	0
2	GOL	T	219	-	5,5,5	0.39	0	5,5,5	1.01	0
2	GOL	R	219	-	5,5,5	0.32	0	5,5,5	0.87	0
2	GOL	Q	219	-	5,5,5	0.46	0	5,5,5	0.93	0
2	GOL	B	219	-	5,5,5	0.41	0	5,5,5	0.88	0
2	GOL	G	219	-	5,5,5	0.83	0	5,5,5	1.35	1 (20%)
2	GOL	E	219	-	5,5,5	0.22	0	5,5,5	0.93	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	J	219	-	-	0/4/4/4	-
2	GOL	A	219	-	-	1/4/4/4	-
2	GOL	K	219[B]	-	-	4/4/4/4	-
2	GOL	L	219	-	-	4/4/4/4	-
2	GOL	I	219	-	-	2/4/4/4	-
2	GOL	O	220	-	-	2/4/4/4	-
2	GOL	C	219	-	-	2/4/4/4	-
2	GOL	K	219[A]	-	-	0/4/4/4	-
2	GOL	F	219	-	-	2/4/4/4	-
2	GOL	D	219	-	-	2/4/4/4	-
2	GOL	H	219	-	-	2/4/4/4	-
2	GOL	P	219	-	-	1/4/4/4	-
2	GOL	N	219	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	M	219	-	-	2/4/4/4	-
2	GOL	S	219	-	-	2/4/4/4	-
2	GOL	P	220	-	-	3/4/4/4	-
2	GOL	T	219	-	-	2/4/4/4	-
2	GOL	R	219	-	-	2/4/4/4	-
2	GOL	Q	219	-	-	2/4/4/4	-
2	GOL	B	219	-	-	0/4/4/4	-
2	GOL	G	219	-	-	3/4/4/4	-
2	GOL	E	219	-	-	0/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	220	GOL	C3-C2-C1	-2.63	102.14	111.80
2	G	219	GOL	O1-C1-C2	2.48	121.56	110.38
2	O	220	GOL	O1-C1-C2	-2.09	100.97	110.38

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	219	GOL	C1-C2-C3-O3
2	F	219	GOL	O1-C1-C2-C3
2	G	219	GOL	C1-C2-C3-O3
2	G	219	GOL	O2-C2-C3-O3
2	H	219	GOL	C1-C2-C3-O3
2	M	219	GOL	C1-C2-C3-O3
2	O	220	GOL	C1-C2-C3-O3
2	P	220	GOL	O1-C1-C2-C3
2	R	219	GOL	O1-C1-C2-C3
2	D	219	GOL	C1-C2-C3-O3
2	I	219	GOL	C1-C2-C3-O3
2	K	219[B]	GOL	O1-C1-C2-C3
2	K	219[B]	GOL	C1-C2-C3-O3
2	L	219	GOL	O1-C1-C2-C3
2	L	219	GOL	C1-C2-C3-O3
2	N	219	GOL	C1-C2-C3-O3
2	Q	219	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	S	219	GOL	C1-C2-C3-O3
2	T	219	GOL	O1-C1-C2-C3
2	C	219	GOL	O2-C2-C3-O3
2	F	219	GOL	O1-C1-C2-O2
2	K	219[B]	GOL	O1-C1-C2-O2
2	L	219	GOL	O1-C1-C2-O2
2	N	219	GOL	O2-C2-C3-O3
2	O	220	GOL	O2-C2-C3-O3
2	P	220	GOL	O1-C1-C2-O2
2	R	219	GOL	O1-C1-C2-O2
2	D	219	GOL	O2-C2-C3-O3
2	H	219	GOL	O2-C2-C3-O3
2	K	219[B]	GOL	O2-C2-C3-O3
2	L	219	GOL	O2-C2-C3-O3
2	M	219	GOL	O2-C2-C3-O3
2	Q	219	GOL	O1-C1-C2-O2
2	G	219	GOL	O1-C1-C2-O2
2	T	219	GOL	O1-C1-C2-O2
2	P	220	GOL	C1-C2-C3-O3
2	A	219	GOL	O2-C2-C3-O3
2	I	219	GOL	O2-C2-C3-O3
2	P	219	GOL	O1-C1-C2-O2
2	S	219	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	219	GOL	1	0
2	O	220	GOL	2	0
2	C	219	GOL	1	0
2	F	219	GOL	1	0
2	H	219	GOL	2	0
2	P	220	GOL	1	0
2	B	219	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	207/230 (90%)	0.56	6 (2%) 53 50	36, 49, 59, 81	0
1	B	209/230 (90%)	0.60	11 (5%) 32 28	39, 49, 67, 79	0
1	C	208/230 (90%)	0.86	11 (5%) 32 28	40, 49, 60, 73	0
1	D	210/230 (91%)	0.24	3 (1%) 73 69	40, 49, 64, 86	0
1	E	216/230 (93%)	0.24	2 (0%) 81 78	41, 49, 60, 75	0
1	F	213/230 (92%)	0.36	4 (1%) 66 62	39, 49, 61, 87	0
1	G	216/230 (93%)	0.52	8 (3%) 45 41	40, 49, 61, 89	0
1	H	205/230 (89%)	0.33	3 (1%) 72 68	38, 49, 60, 70	0
1	I	211/230 (91%)	0.30	7 (3%) 49 45	41, 48, 60, 83	0
1	J	213/230 (92%)	0.82	18 (8%) 16 13	37, 49, 72, 83	0
1	K	216/230 (93%)	0.43	2 (0%) 81 78	39, 48, 61, 69	0
1	L	204/230 (88%)	0.34	2 (0%) 79 76	37, 48, 57, 85	0
1	M	198/230 (86%)	0.54	8 (4%) 42 38	40, 48, 60, 68	0
1	N	204/230 (88%)	0.85	13 (6%) 25 22	40, 48, 57, 66	0
1	O	210/230 (91%)	0.39	5 (2%) 59 55	39, 48, 65, 82	0
1	P	209/230 (90%)	0.21	2 (0%) 79 76	39, 49, 60, 84	0
1	Q	208/230 (90%)	0.26	7 (3%) 48 44	24, 48, 60, 74	1 (0%)
1	R	210/230 (91%)	0.69	15 (7%) 22 18	40, 49, 61, 74	0
1	S	205/230 (89%)	0.57	5 (2%) 59 55	40, 48, 60, 72	0
1	T	204/230 (88%)	0.63	9 (4%) 39 34	40, 48, 57, 66	0
All	All	4176/4600 (90%)	0.49	141 (3%) 48 44	24, 49, 61, 89	1 (0%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	T	205	PHE	4.4
1	J	209	TRP	4.4
1	N	206	MET	4.3
1	A	41	GLN	4.3
1	A	216	LEU	4.0
1	H	32	ILE	3.9
1	D	205	PHE	3.6
1	C	205	PHE	3.6
1	J	31	LEU	3.6
1	A	29	PRO	3.5
1	B	206	MET	3.5
1	B	205	PHE	3.4
1	J	29	PRO	3.4
1	M	8	ALA	3.4
1	B	207	GLU	3.4
1	I	58	VAL	3.3
1	B	203	GLU	3.3
1	A	-1	HIS	3.2
1	G	205	PHE	3.2
1	O	-1	HIS	3.1
1	C	142	ARG	3.1
1	R	70	ALA	3.1
1	K	0	HIS	3.0
1	G	-1	HIS	3.0
1	N	61	LEU	3.0
1	C	45	GLU	2.9
1	P	207	GLU	2.9
1	B	-1	HIS	2.9
1	I	21	ILE	2.9
1	O	205	PHE	2.9
1	D	-1	HIS	2.9
1	R	213	LEU	2.9
1	J	33	SER	2.8
1	J	37	ALA	2.8
1	J	32	ILE	2.8
1	S	31	LEU	2.8
1	M	91	ILE	2.8
1	C	58	VAL	2.8
1	C	16	GLY	2.8
1	N	8	ALA	2.8
1	N	187	ALA	2.7
1	J	36	GLY	2.7
1	R	209	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	R	215	ASN	2.7
1	Q	209	TRP	2.7
1	N	47	CYS	2.7
1	J	78	GLU	2.7
1	D	21	ILE	2.6
1	E	215	ASN	2.6
1	M	58	VAL	2.6
1	T	27	THR	2.6
1	N	39	PHE	2.6
1	R	205	PHE	2.6
1	F	216	LEU	2.6
1	C	0	HIS	2.6
1	F	-1	HIS	2.6
1	O	10	LEU	2.5
1	B	202	ILE	2.5
1	M	116	ILE	2.5
1	I	39	PHE	2.5
1	I	214	GLU	2.5
1	Q	28	ASN	2.5
1	B	33	SER	2.5
1	G	214	GLU	2.4
1	N	46	ILE	2.4
1	H	0	HIS	2.4
1	H	29	PRO	2.4
1	R	52	GLY	2.4
1	B	199	ASP	2.4
1	R	0	HIS	2.4
1	Q	179	VAL	2.4
1	B	21	ILE	2.4
1	T	21	ILE	2.4
1	T	48	ASP	2.4
1	J	59	VAL	2.4
1	Q	210	LYS	2.4
1	N	205	PHE	2.3
1	N	54	VAL	2.3
1	G	142	ARG	2.3
1	M	204	ARG	2.3
1	K	209	TRP	2.3
1	I	-1	HIS	2.3
1	N	0	HIS	2.3
1	O	28	ASN	2.3
1	T	30	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	R	206	MET	2.3
1	B	18	GLU	2.3
1	C	35	GLU	2.3
1	B	116	ILE	2.2
1	F	209	TRP	2.2
1	G	18	GLU	2.2
1	Q	214	GLU	2.2
1	J	20	GLY	2.2
1	L	206	MET	2.2
1	G	32	ILE	2.2
1	A	6	ASP	2.2
1	M	203	GLU	2.2
1	M	59	VAL	2.2
1	J	7	THR	2.2
1	L	21	ILE	2.2
1	J	156	PHE	2.2
1	Q	205	PHE	2.2
1	P	-1	HIS	2.2
1	N	21	ILE	2.2
1	R	59	VAL	2.1
1	J	121	ALA	2.1
1	R	121	ALA	2.1
1	S	121	ALA	2.1
1	J	10	LEU	2.1
1	R	200	LEU	2.1
1	M	32	ILE	2.1
1	R	21	ILE	2.1
1	C	207	GLU	2.1
1	R	8	ALA	2.1
1	G	213	LEU	2.1
1	N	49	LEU	2.1
1	R	82	ILE	2.1
1	C	18	GLU	2.1
1	E	0	HIS	2.1
1	N	193	PHE	2.1
1	A	8	ALA	2.1
1	O	31	LEU	2.1
1	J	207	GLU	2.1
1	T	45	GLU	2.1
1	F	29	PRO	2.1
1	C	206	MET	2.1
1	T	213	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	116	ILE	2.1
1	Q	155	GLY	2.0
1	T	16	GLY	2.0
1	I	33	SER	2.0
1	I	206	MET	2.0
1	J	-1	HIS	2.0
1	T	75	GLN	2.0
1	S	59	VAL	2.0
1	S	204	ARG	2.0
1	C	32	ILE	2.0
1	G	48	ASP	2.0
1	J	88	PRO	2.0
1	R	212	TYR	2.0
1	S	0	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	O	219	5/5	0.61	0.17	91,92,96,103	0
2	GOL	N	219	6/6	0.66	0.19	61,67,68,74	0
2	GOL	G	219	6/6	0.68	0.23	34,49,53,57	0
2	GOL	E	219	6/6	0.75	0.18	33,49,51,65	0
2	GOL	H	219	6/6	0.75	0.19	49,55,58,65	0
2	GOL	S	219	6/6	0.76	0.17	61,65,67,70	0
2	GOL	R	219	6/6	0.76	0.19	61,70,76,81	0
2	GOL	F	219	6/6	0.77	0.15	60,62,62,69	0
2	GOL	Q	219	6/6	0.79	0.20	44,52,62,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	O	220	6/6	0.79	0.17	47,49,53,62	0
2	GOL	L	219	6/6	0.80	0.15	85,90,93,94	0
2	GOL	P	220	6/6	0.80	0.20	45,54,59,59	0
2	GOL	C	219	6/6	0.80	0.16	58,60,68,71	0
2	GOL	D	219	6/6	0.81	0.17	52,58,64,65	0
2	GOL	T	219	6/6	0.82	0.14	54,67,71,74	0
2	GOL	P	219	6/6	0.82	0.17	54,73,81,85	0
2	GOL	M	219	6/6	0.83	0.16	74,77,77,81	0
2	GOL	J	219	6/6	0.83	0.16	42,53,62,68	0
2	GOL	K	219[B]	6/6	0.84	0.14	34,45,48,53	4
2	GOL	K	219[A]	6/6	0.84	0.14	38,46,48,53	4
2	GOL	B	219	6/6	0.85	0.18	41,55,67,68	0
2	GOL	A	219	6/6	0.86	0.15	42,57,58,58	0
2	GOL	I	219	6/6	0.88	0.14	51,56,59,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.